

Supporting Information

Facile one-pot three-component synthesis of diverse 2,3-disubstituted isoindolin-1-ones using ZrO₂ nanoparticles as a reusable dual acid-base solid support under solvent-free conditions

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Reaction Scheme:

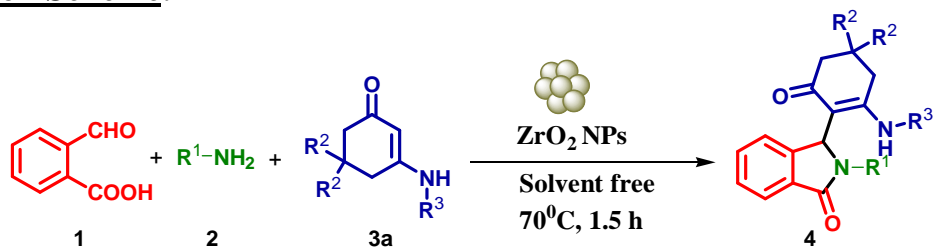
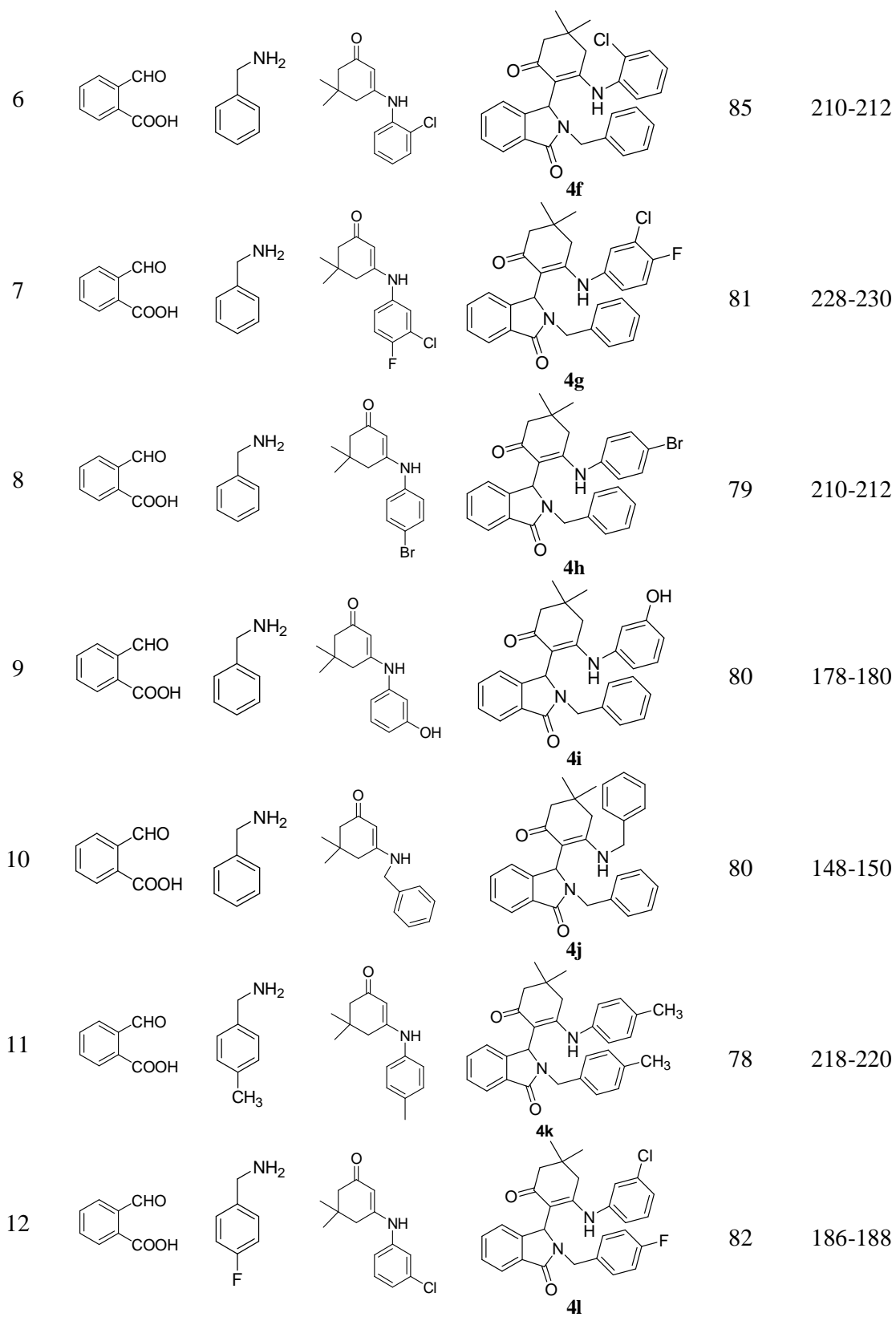
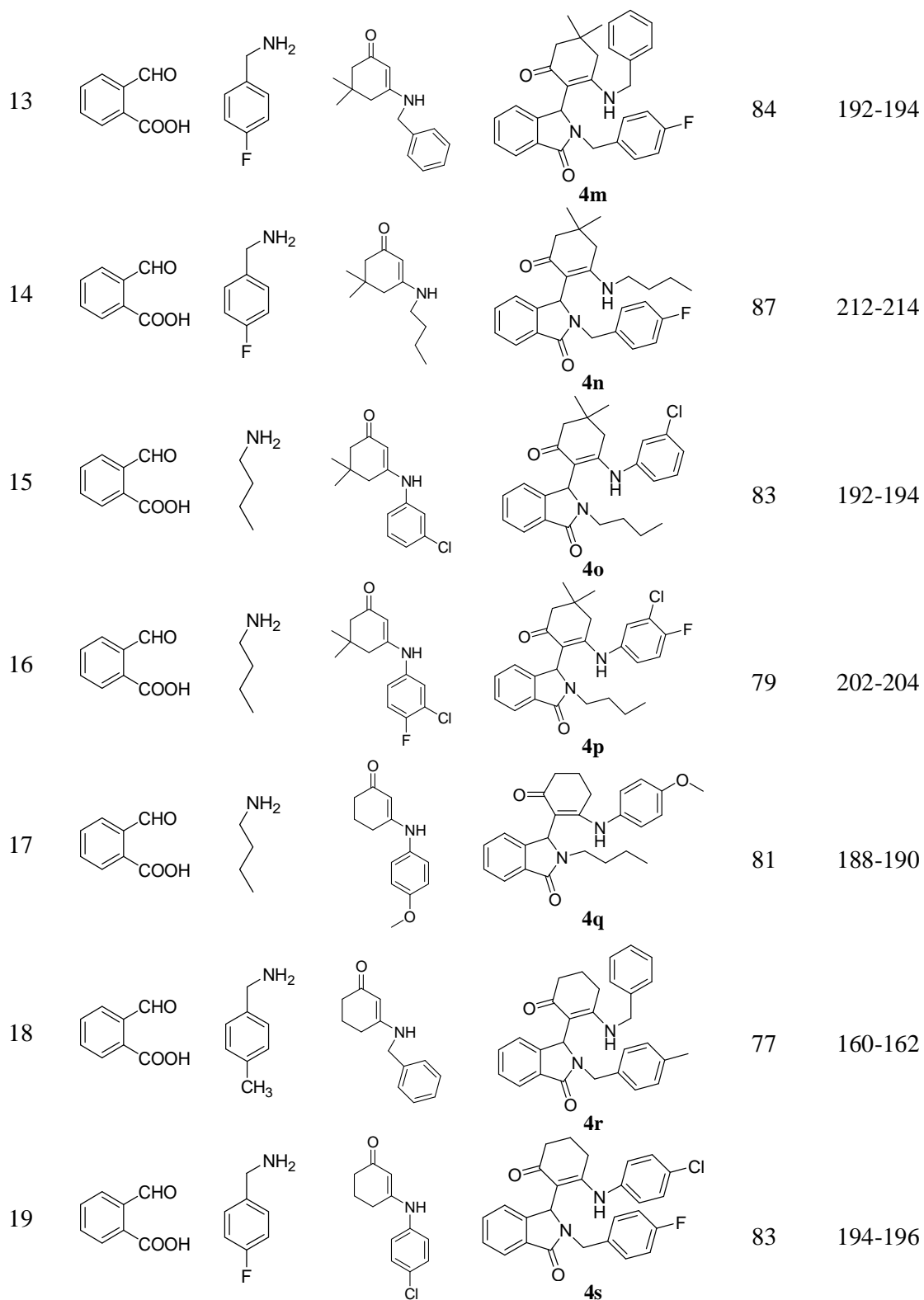
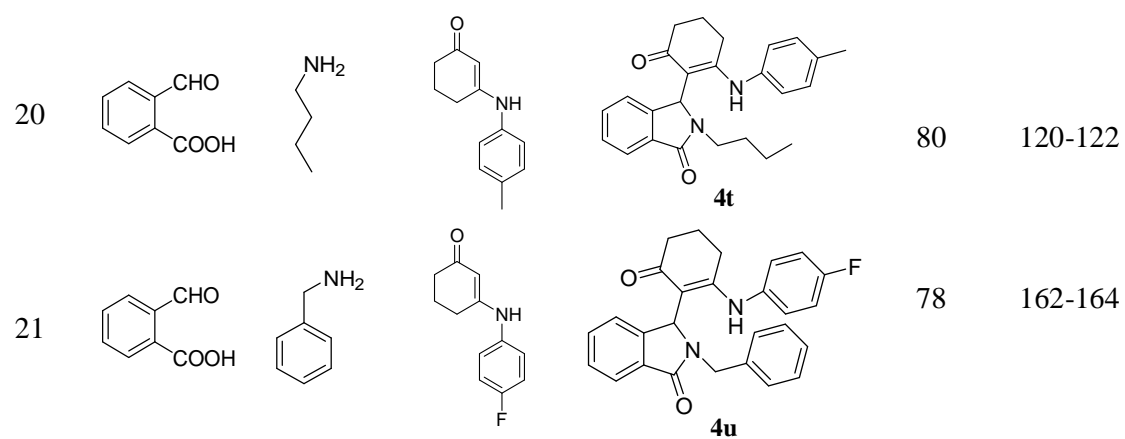


Table S1: Synthesis of 2,3-disubstituted isoindolin-1-ones **4a-s** through a three-component reaction

Entry	1	2	3a	4	Yield (%) ^a	Melting Point (°C)
1					87	160-162
2					85	148-150
3					86	182-184
4					90	190-192
5					88	220-222

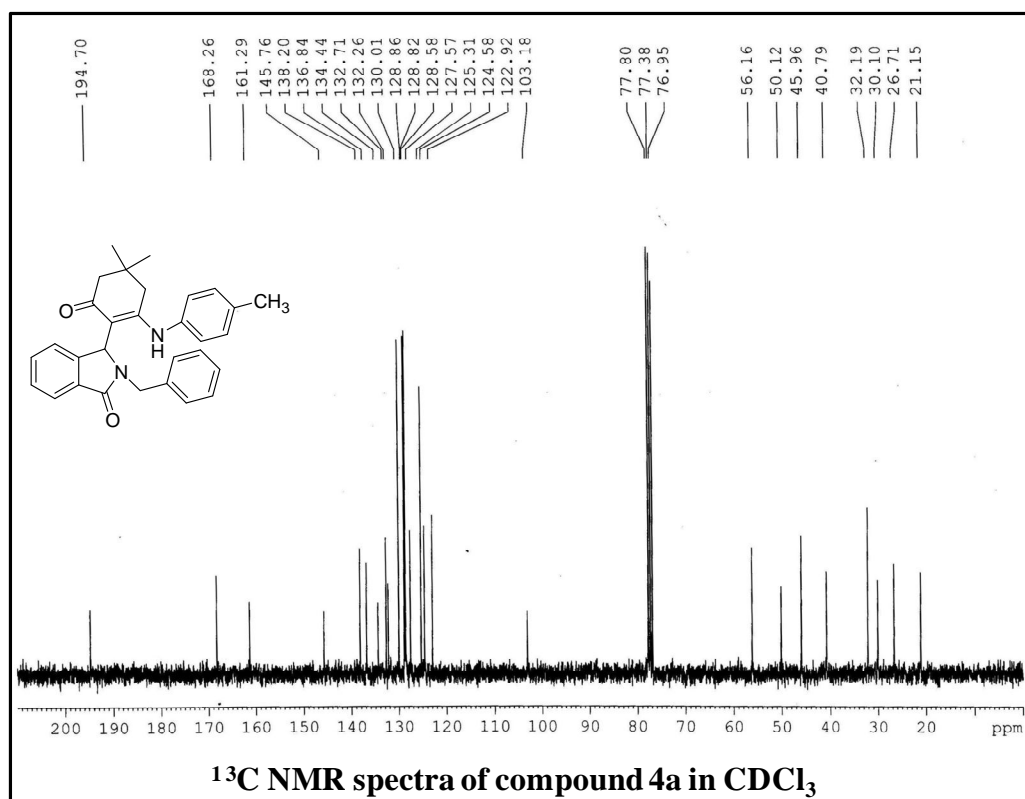
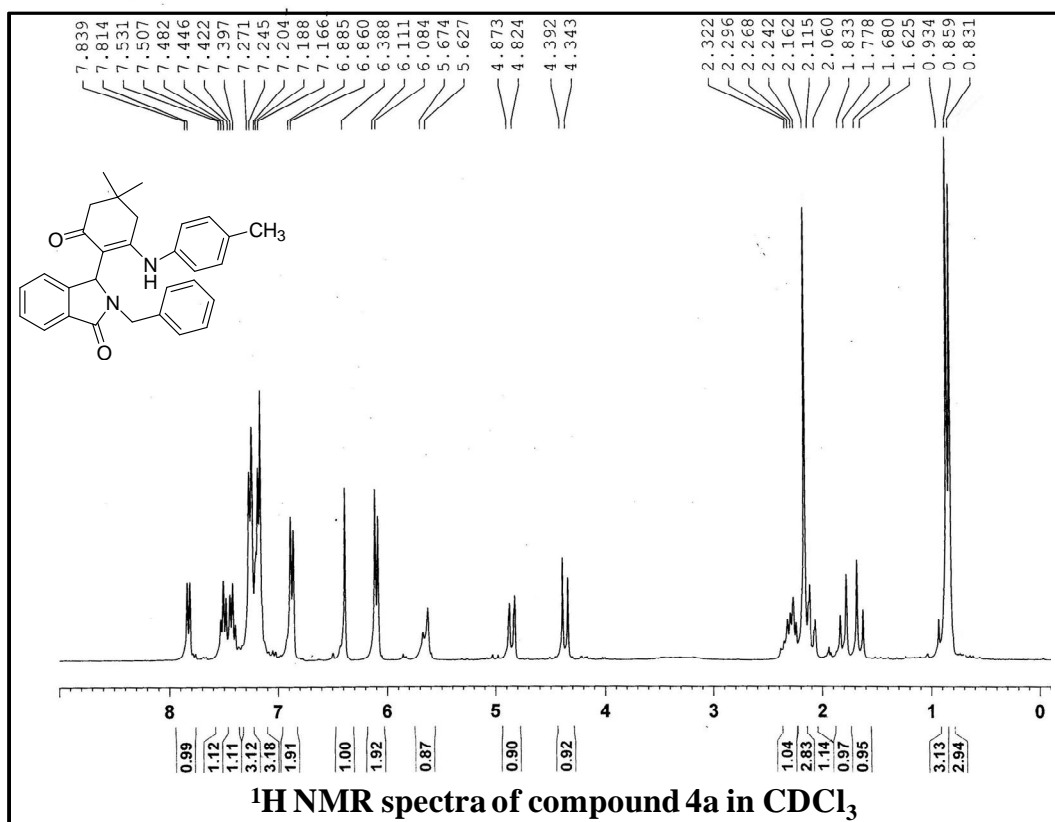


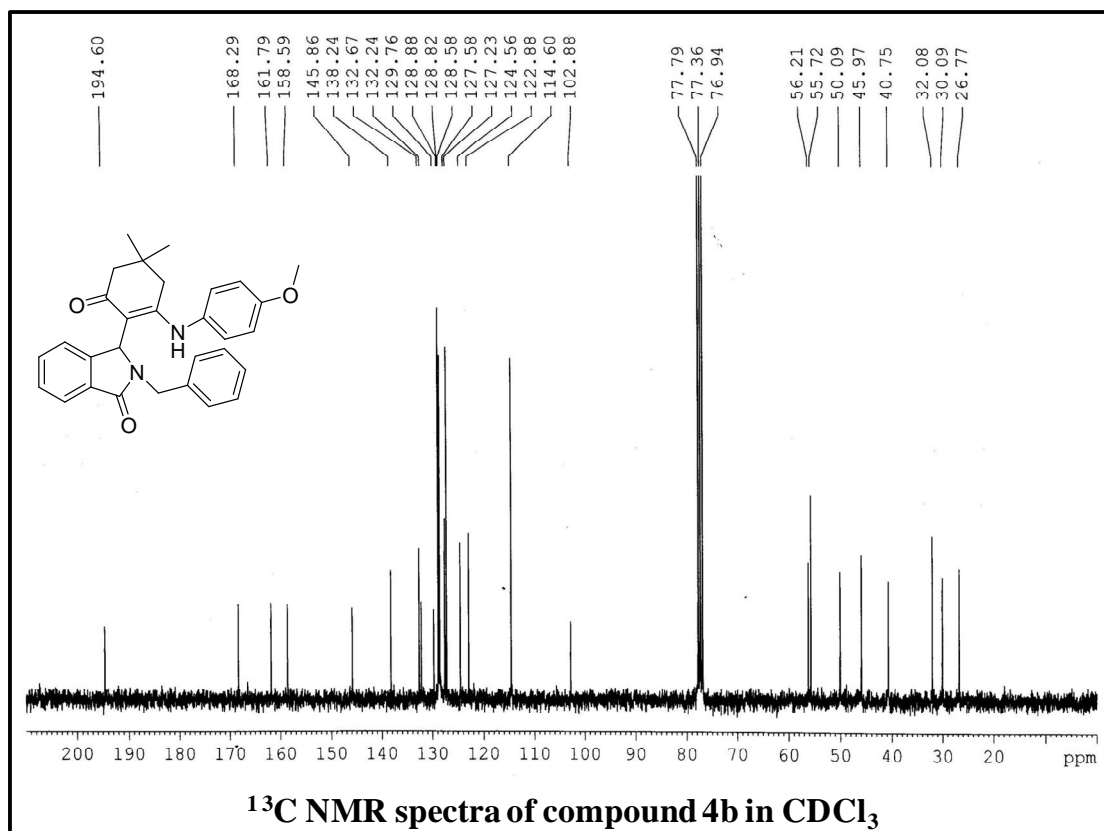
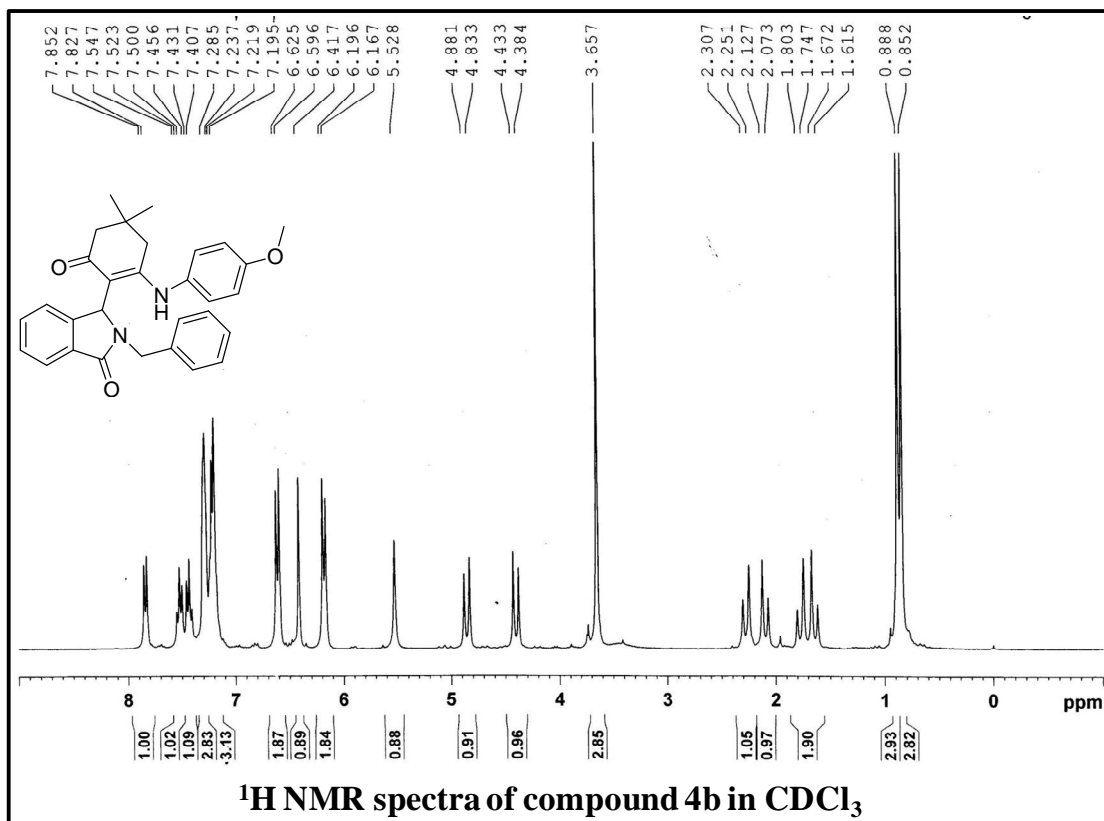


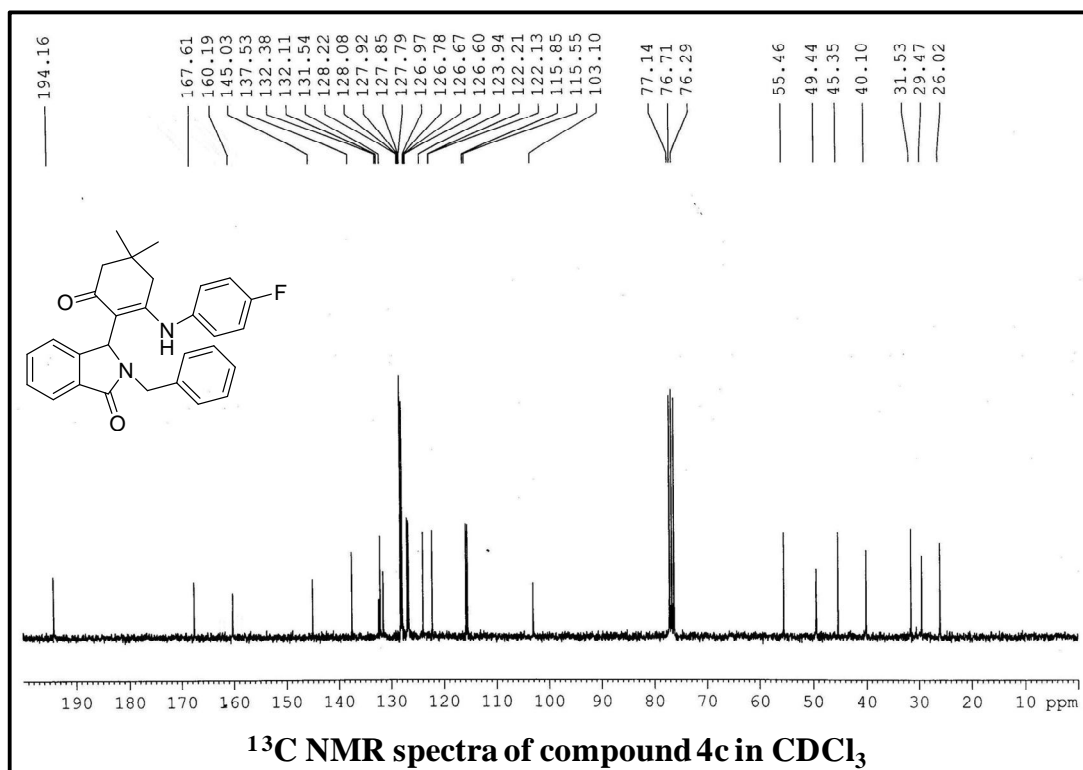
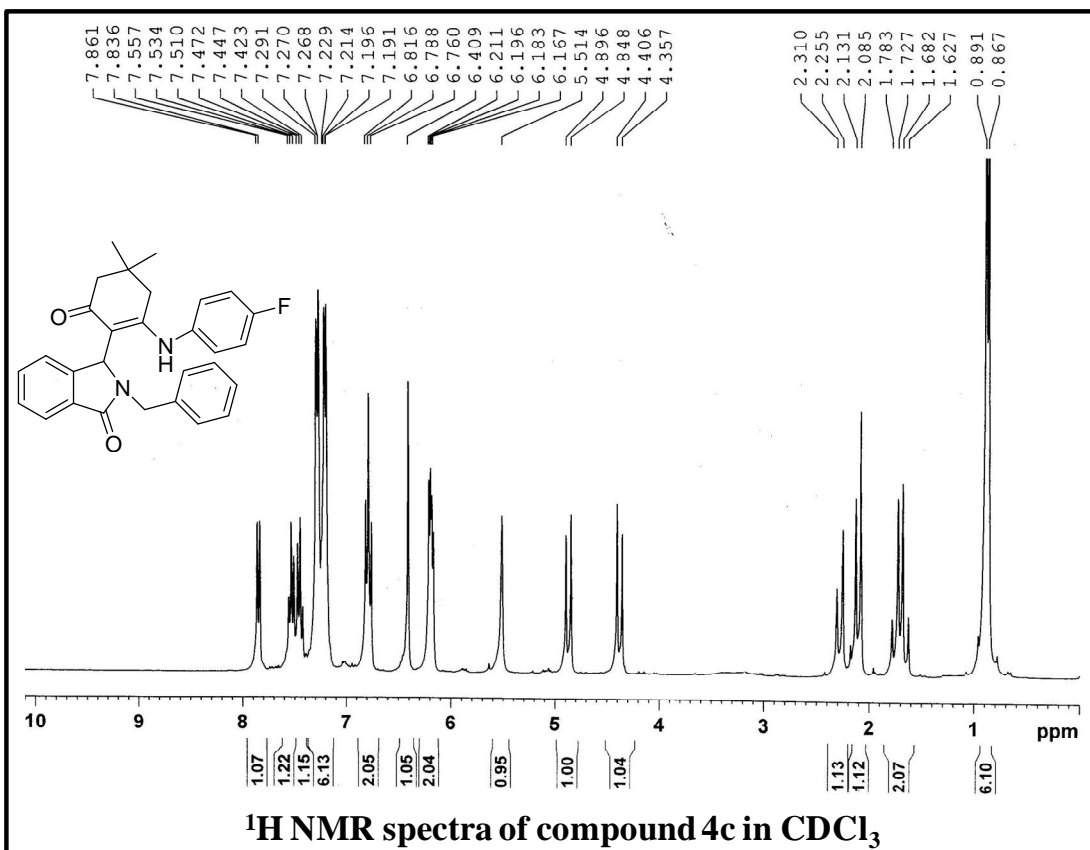


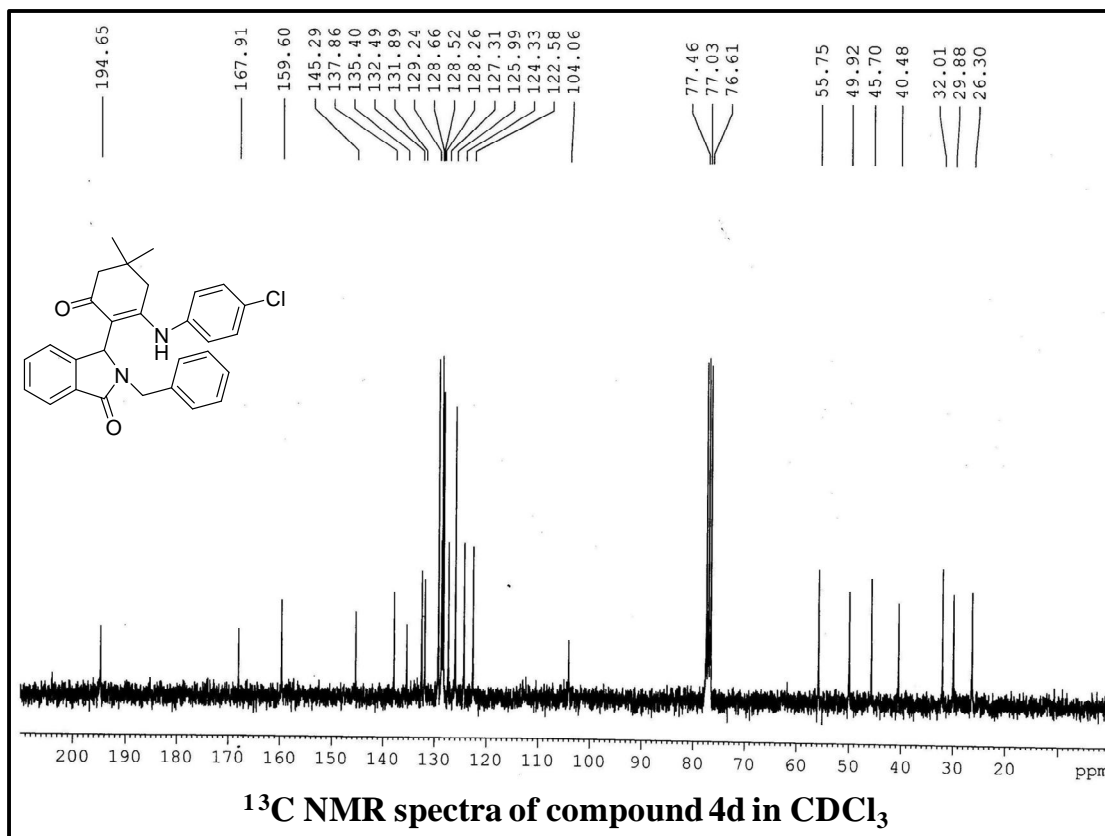
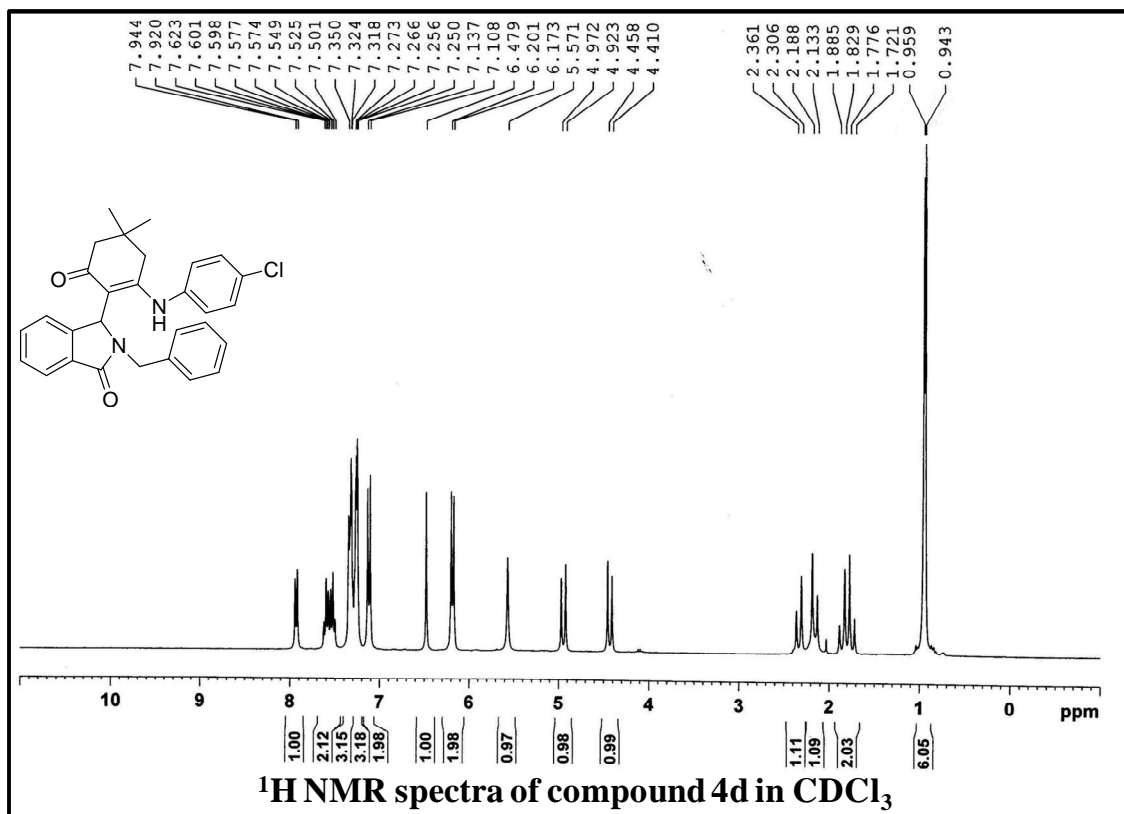
^aIsolated Yields (%)

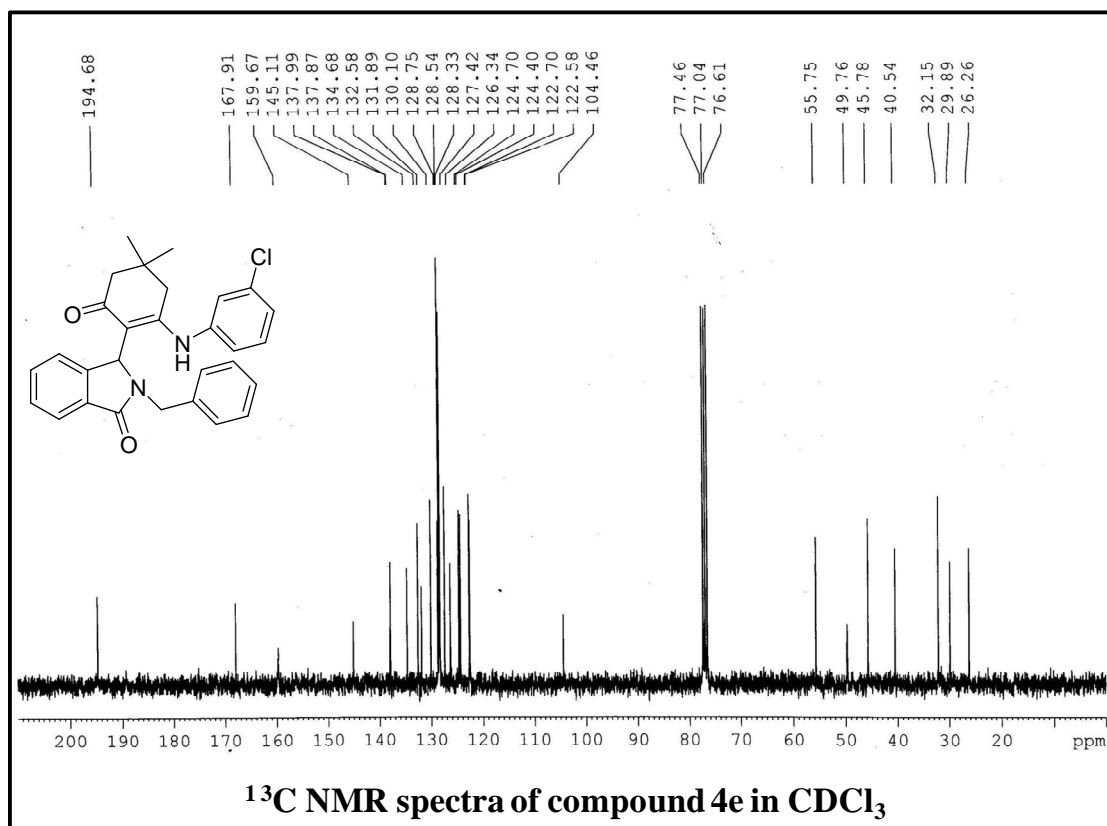
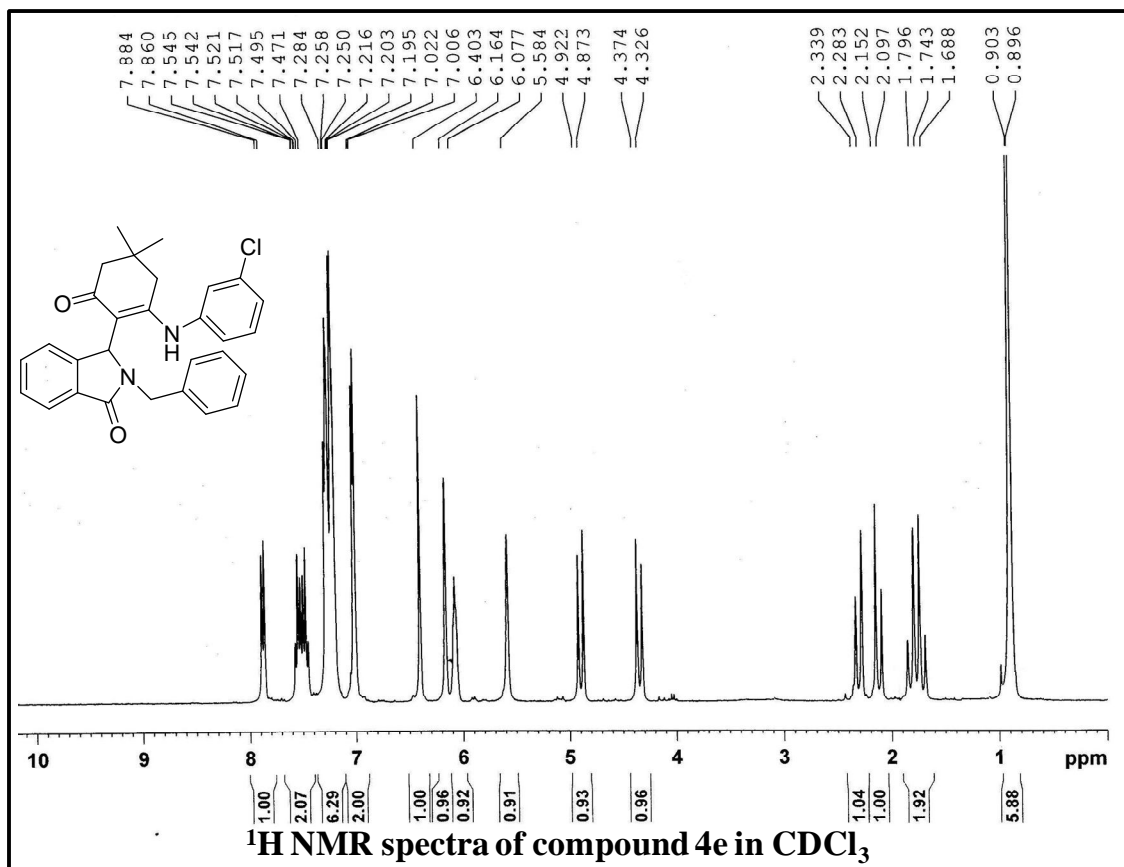
Spectral Data of 4a-u:

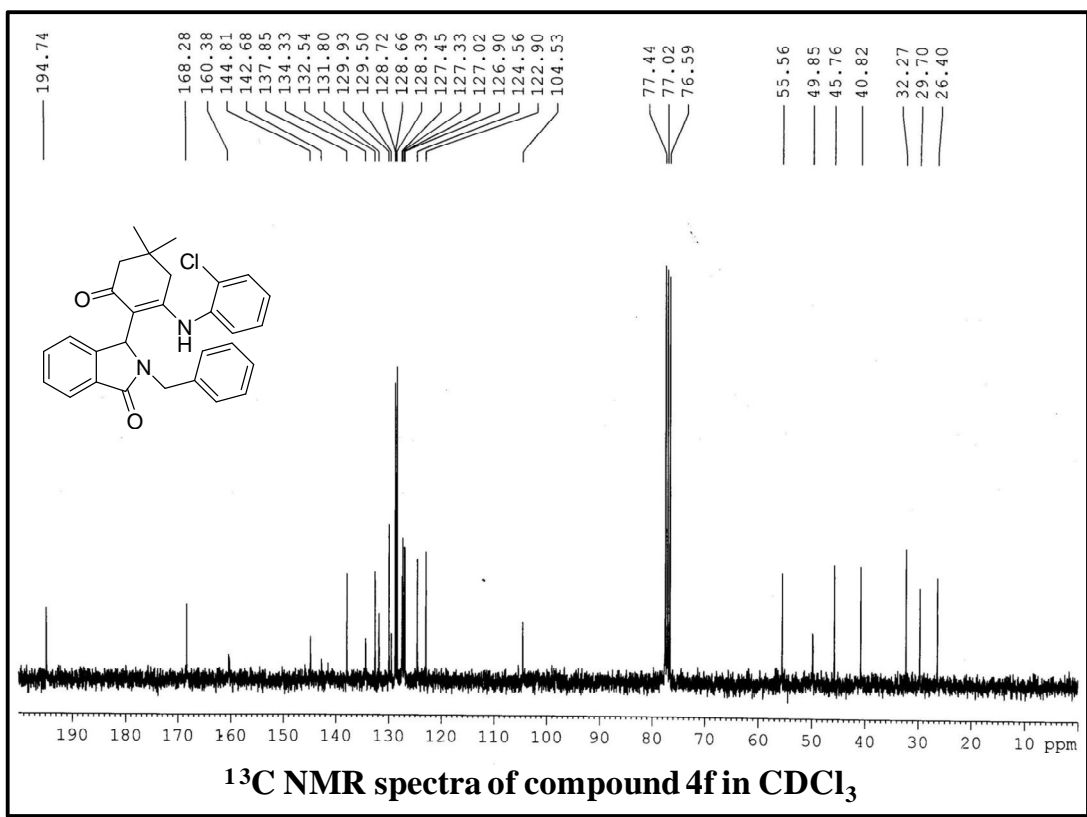
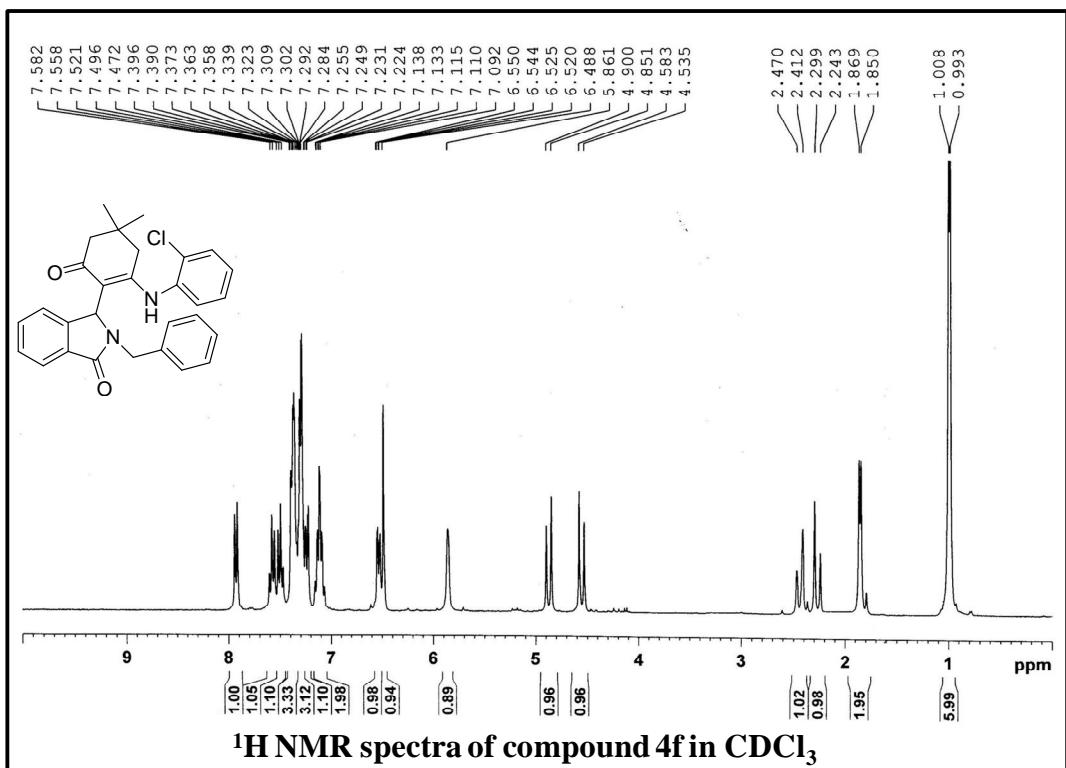


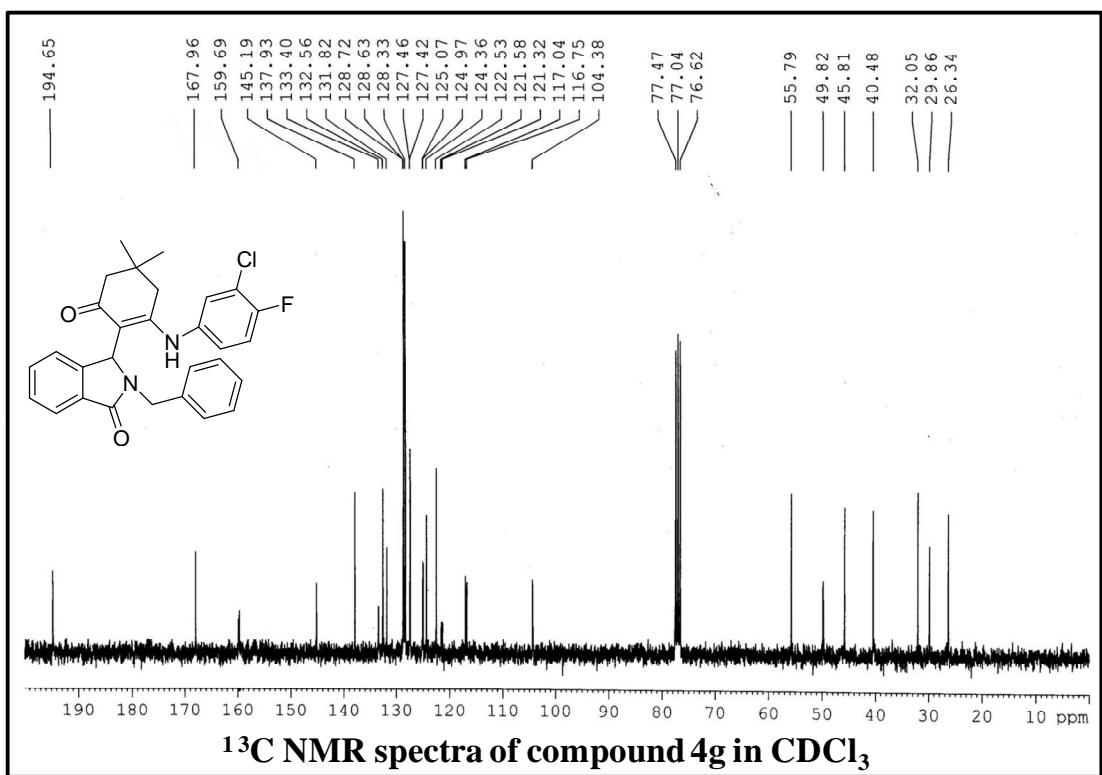
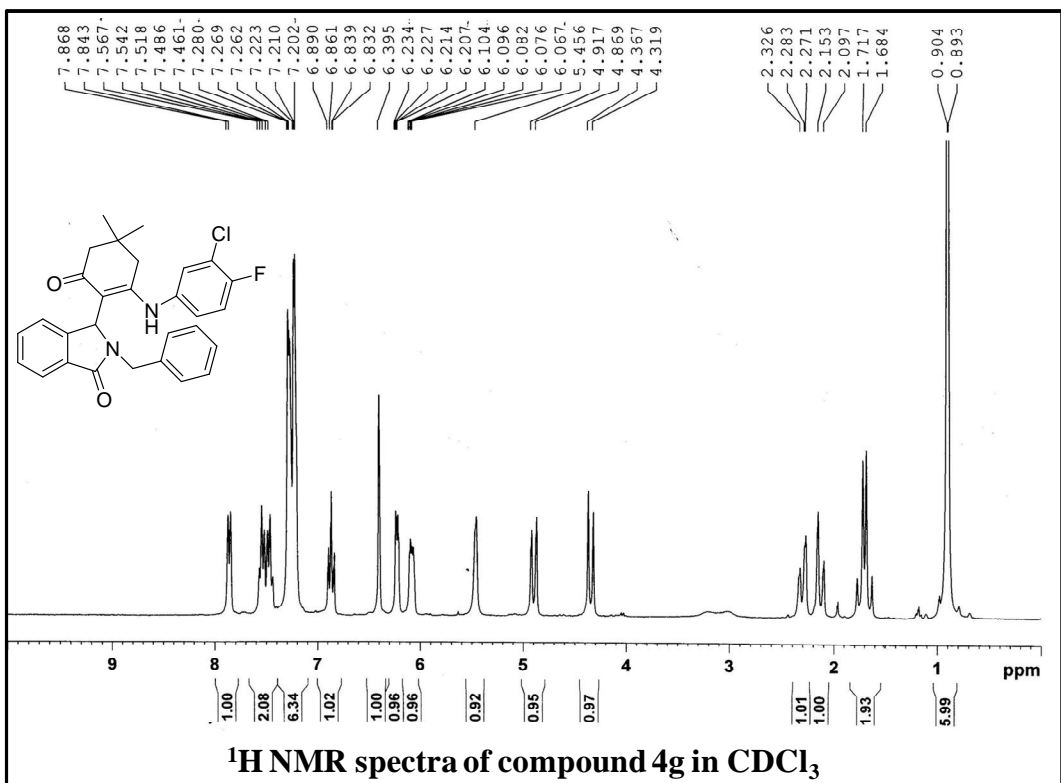


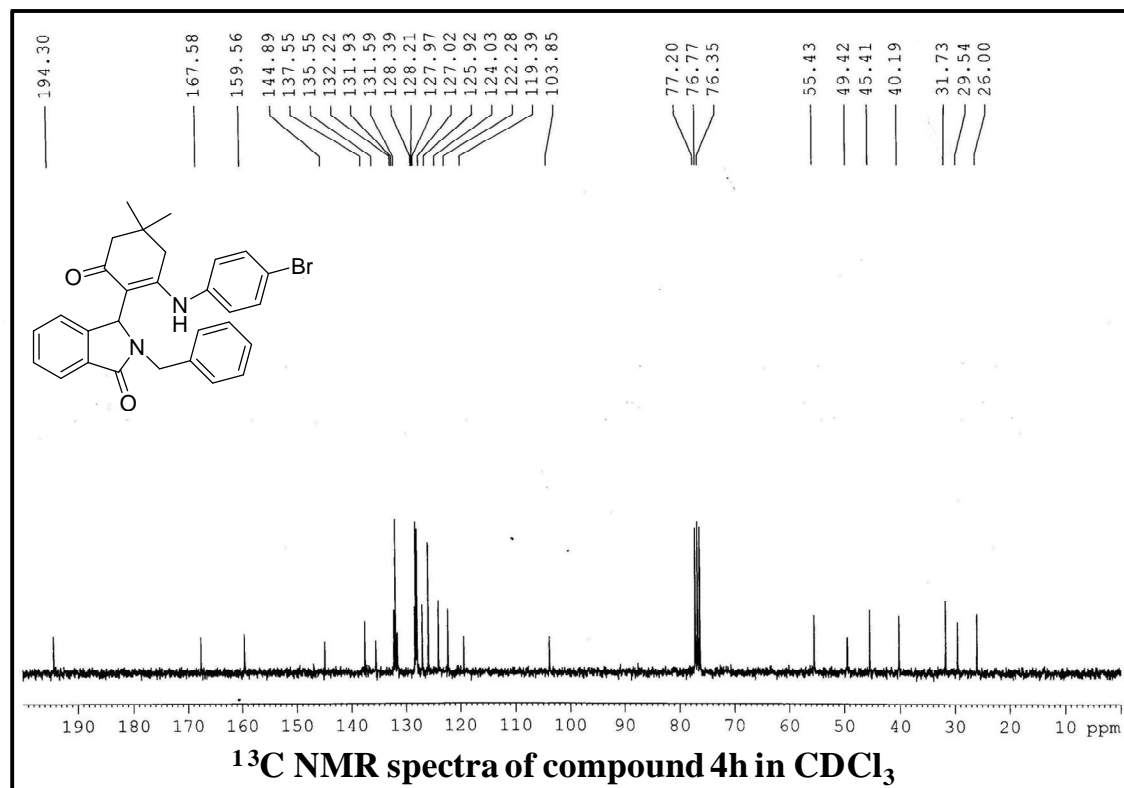
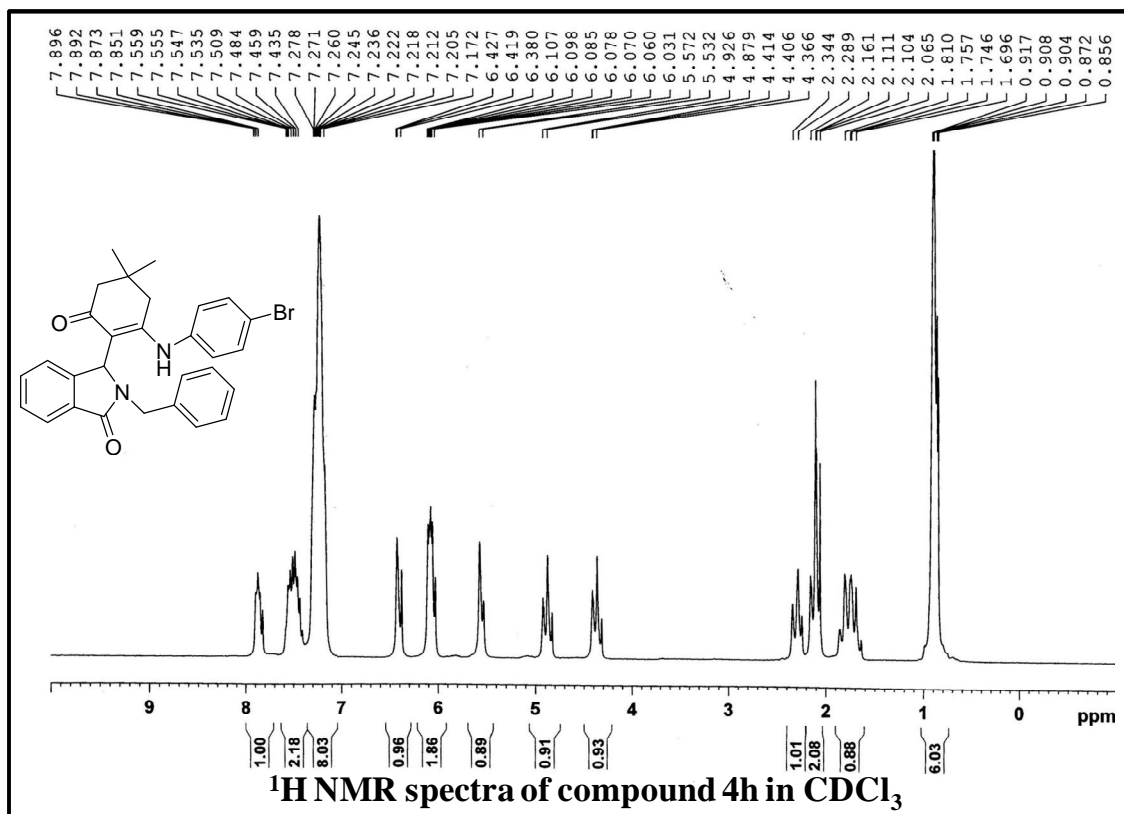


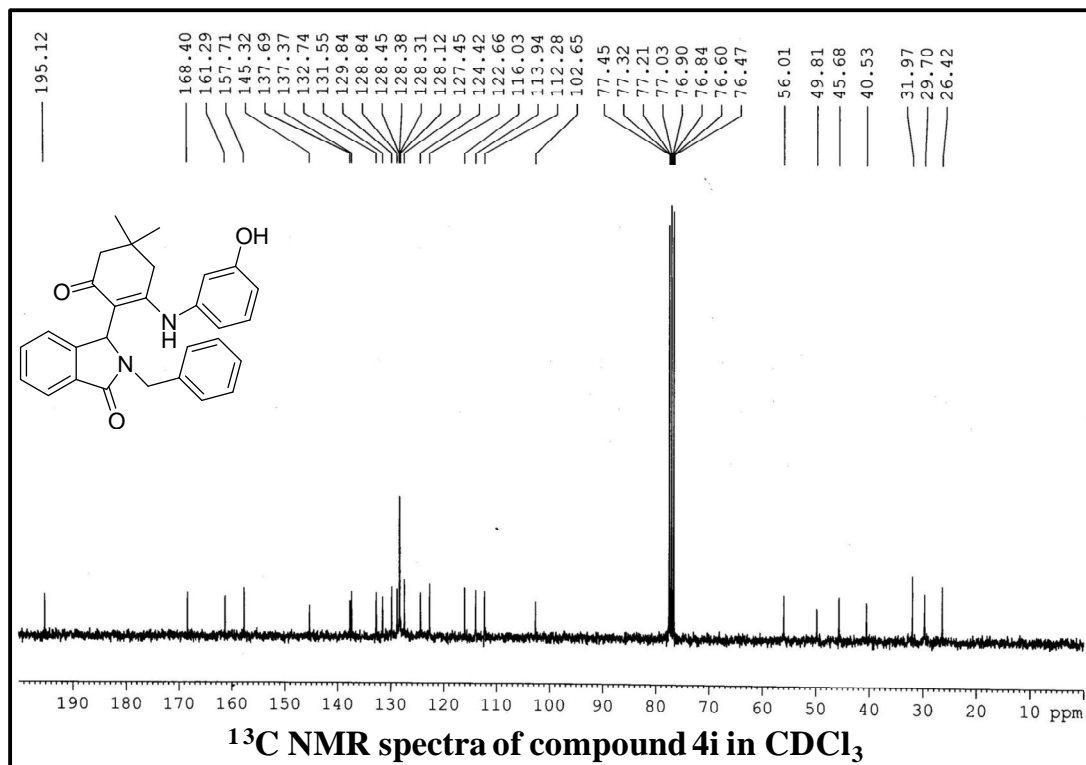
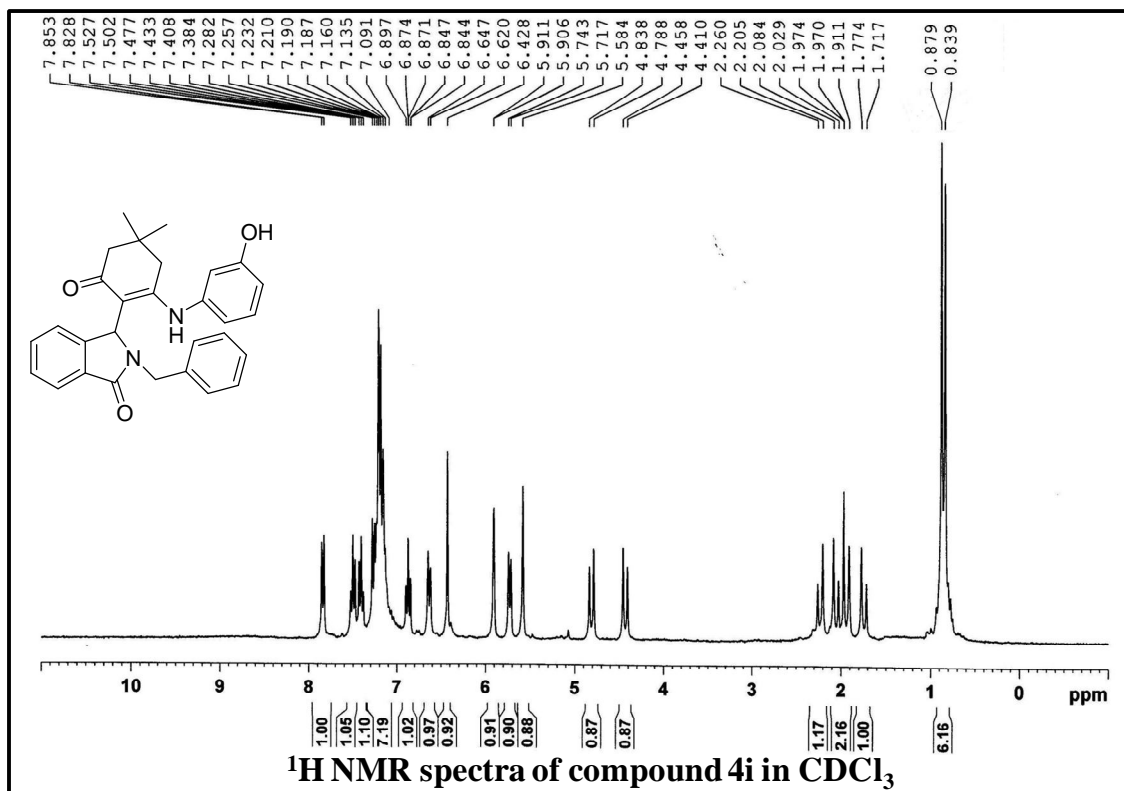


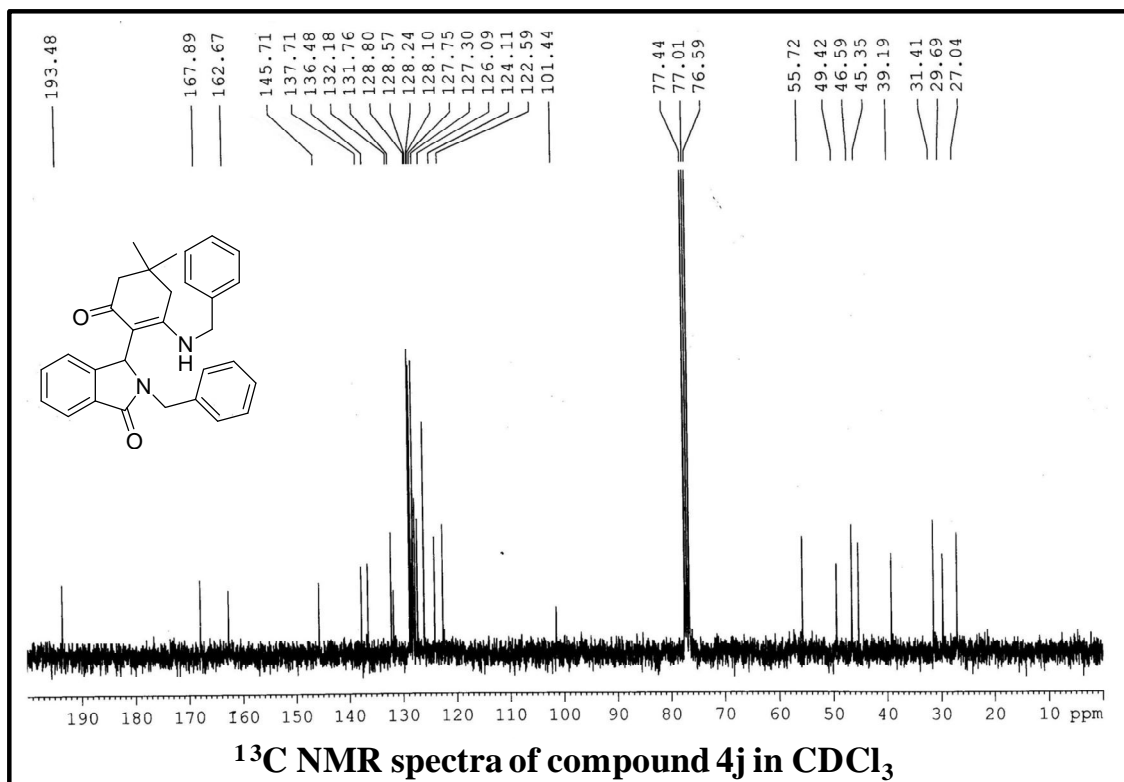
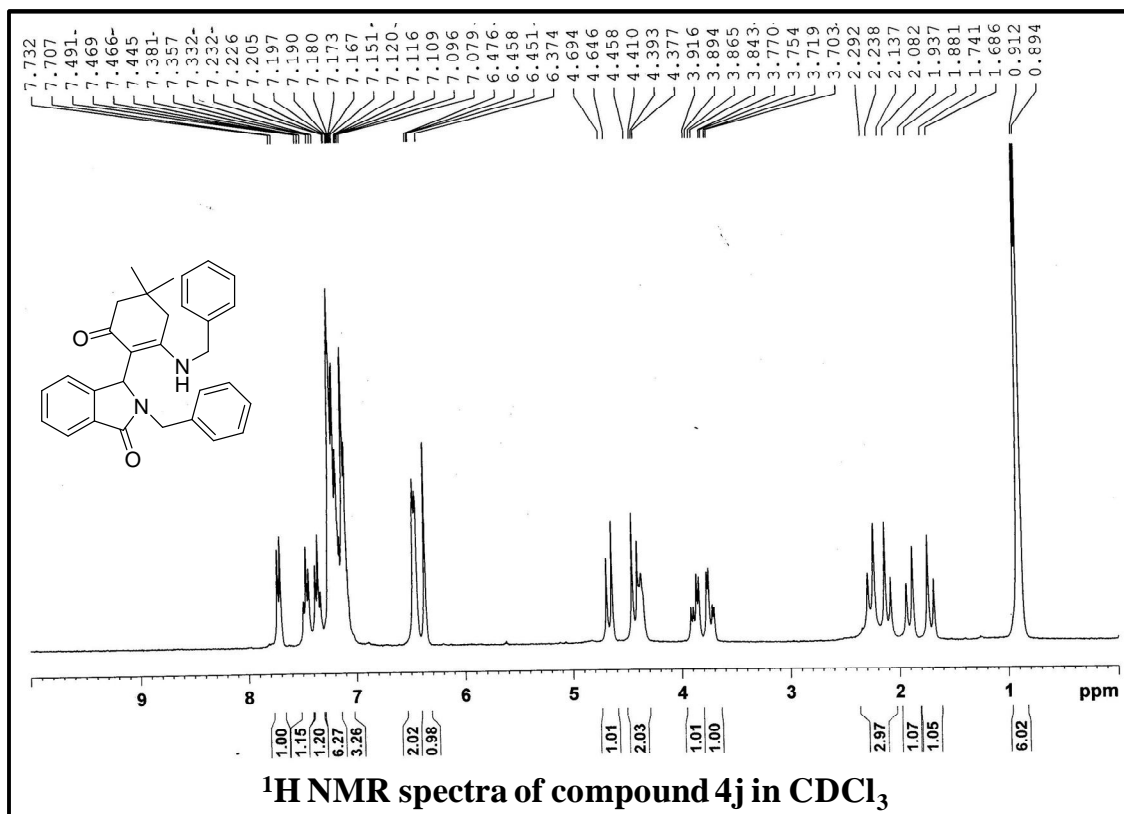


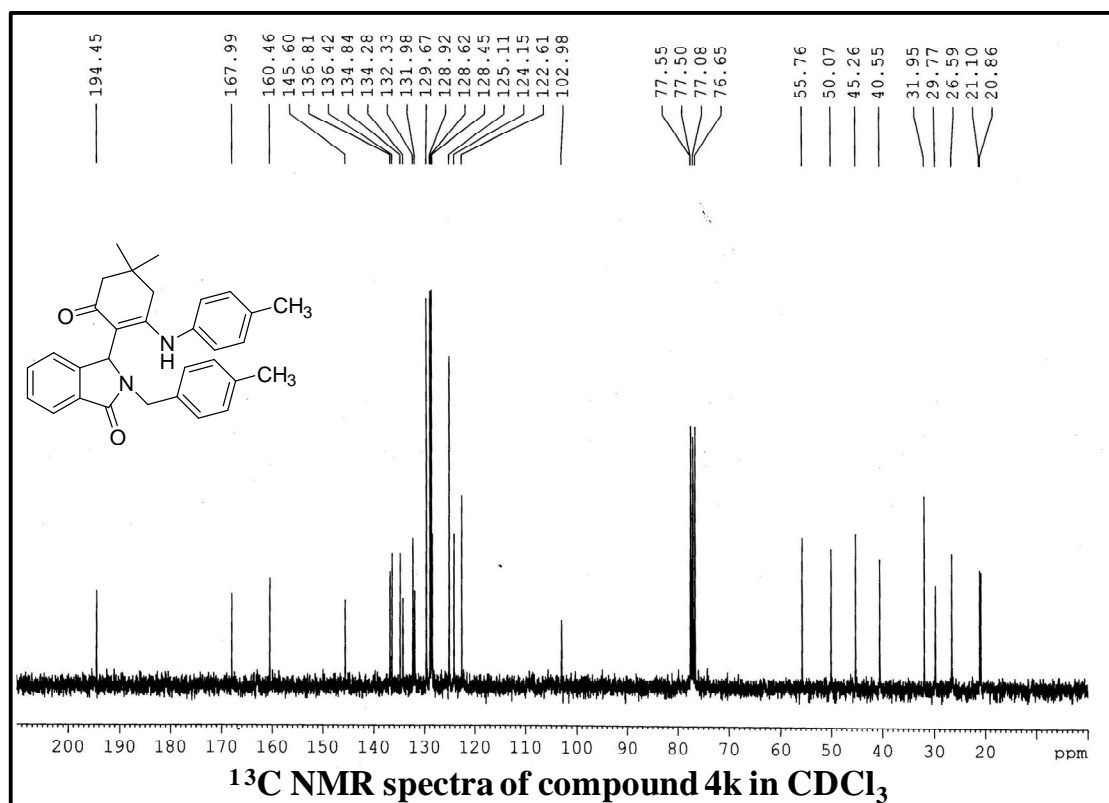
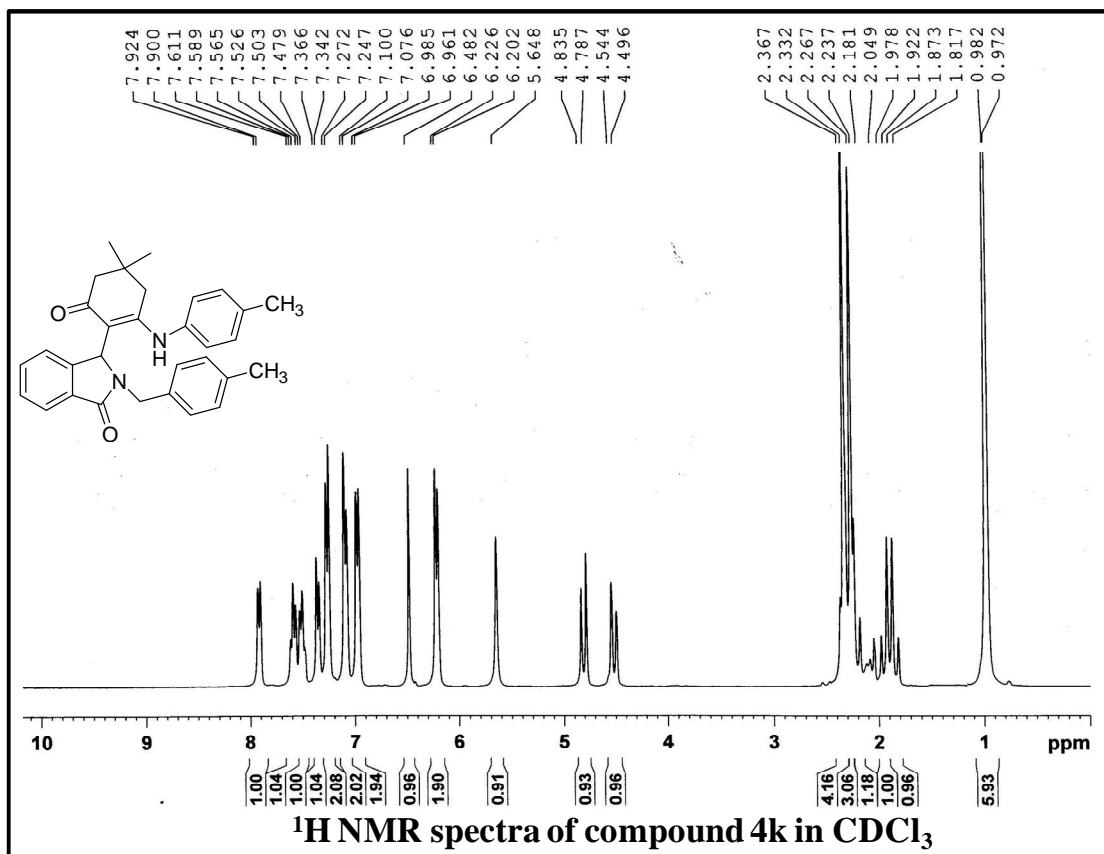


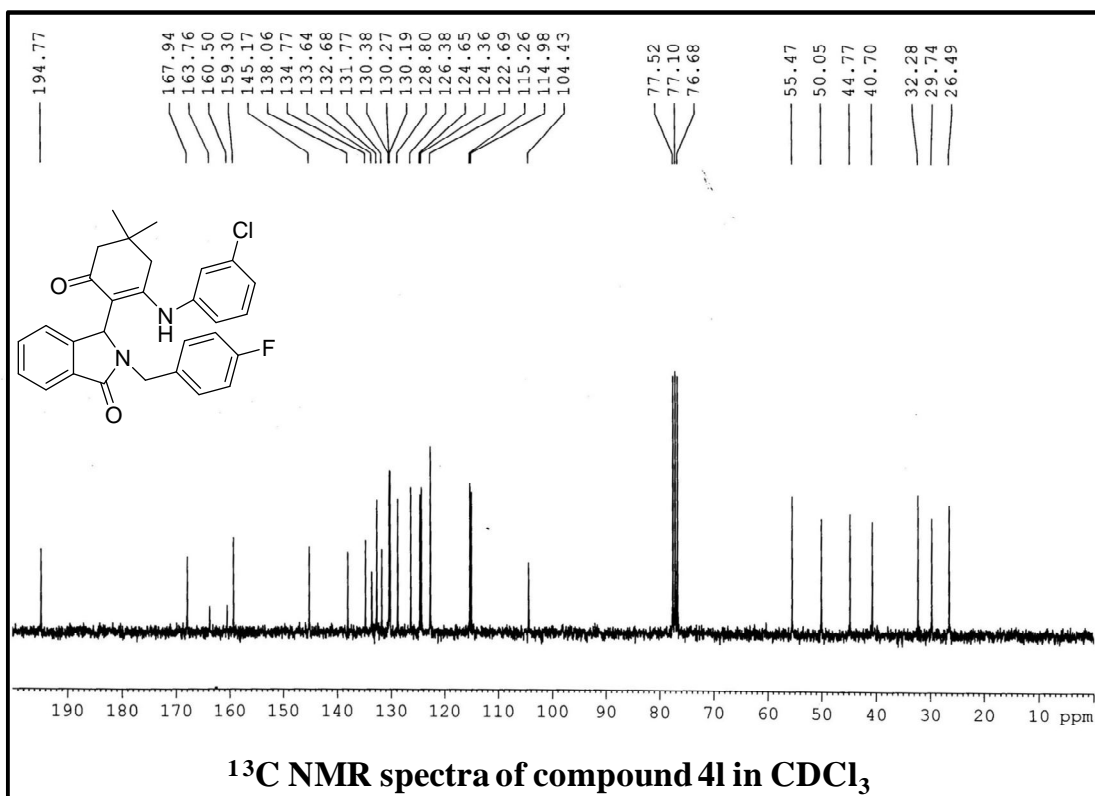
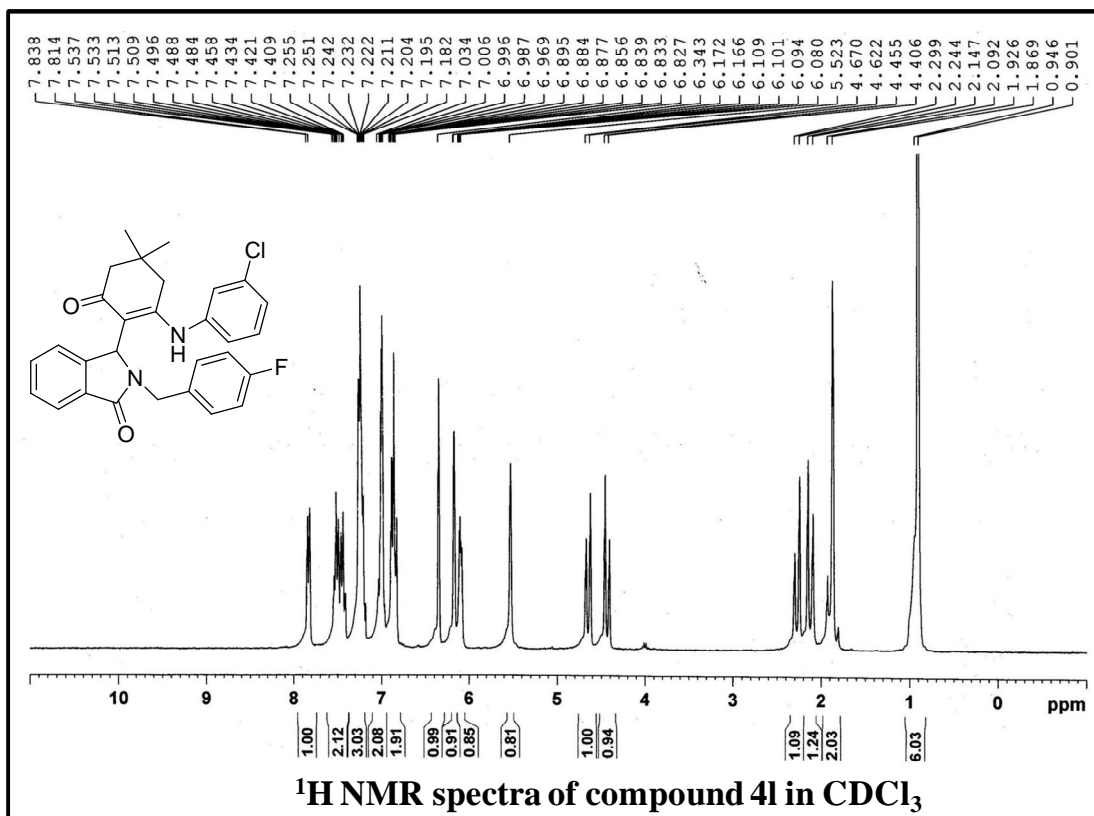


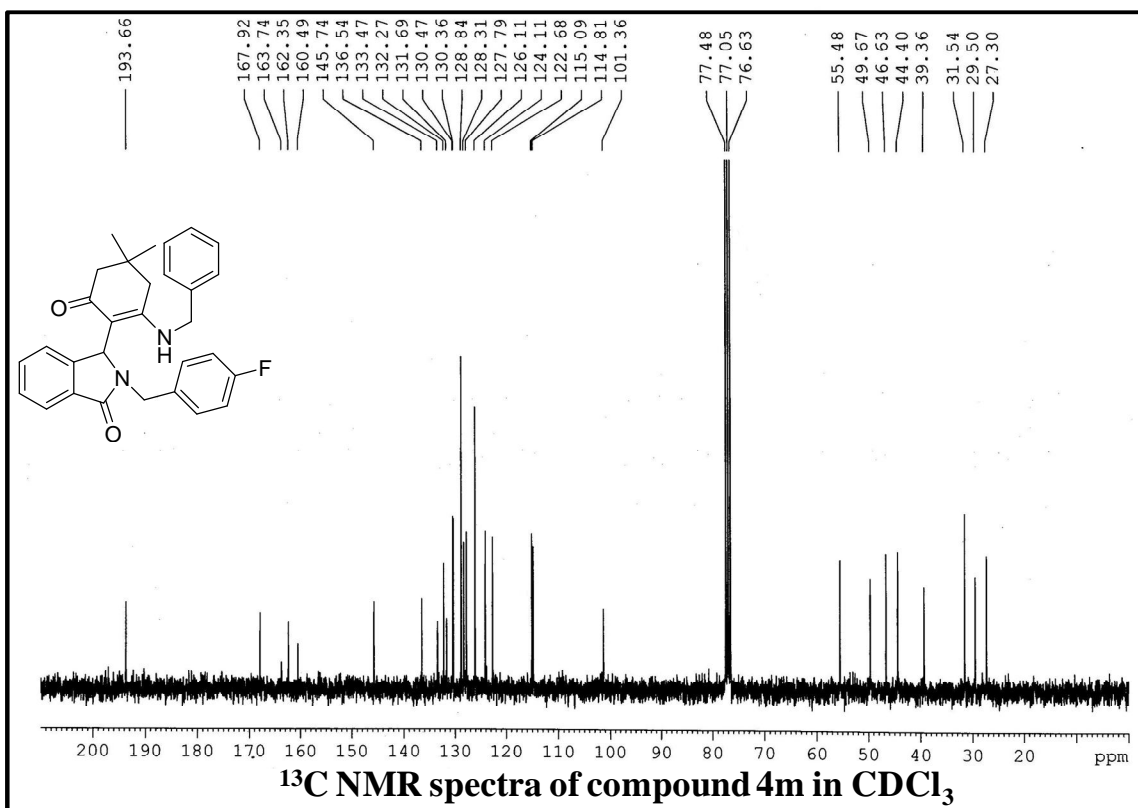
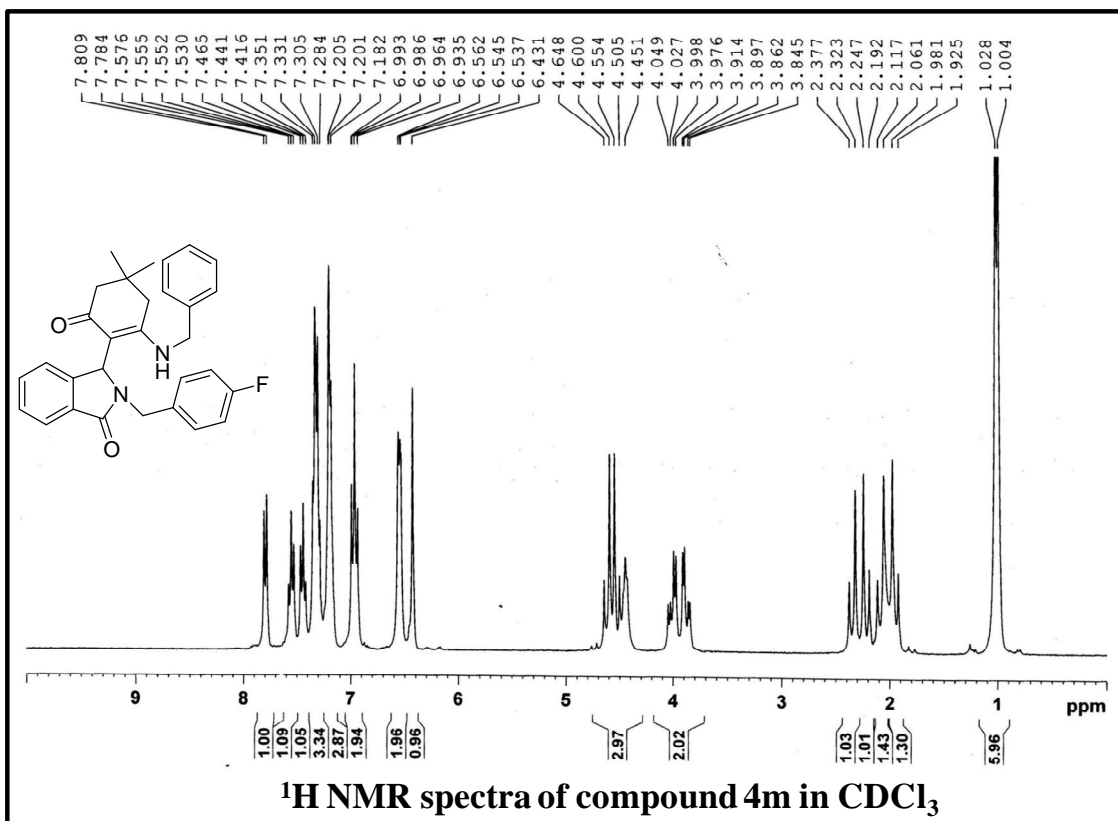


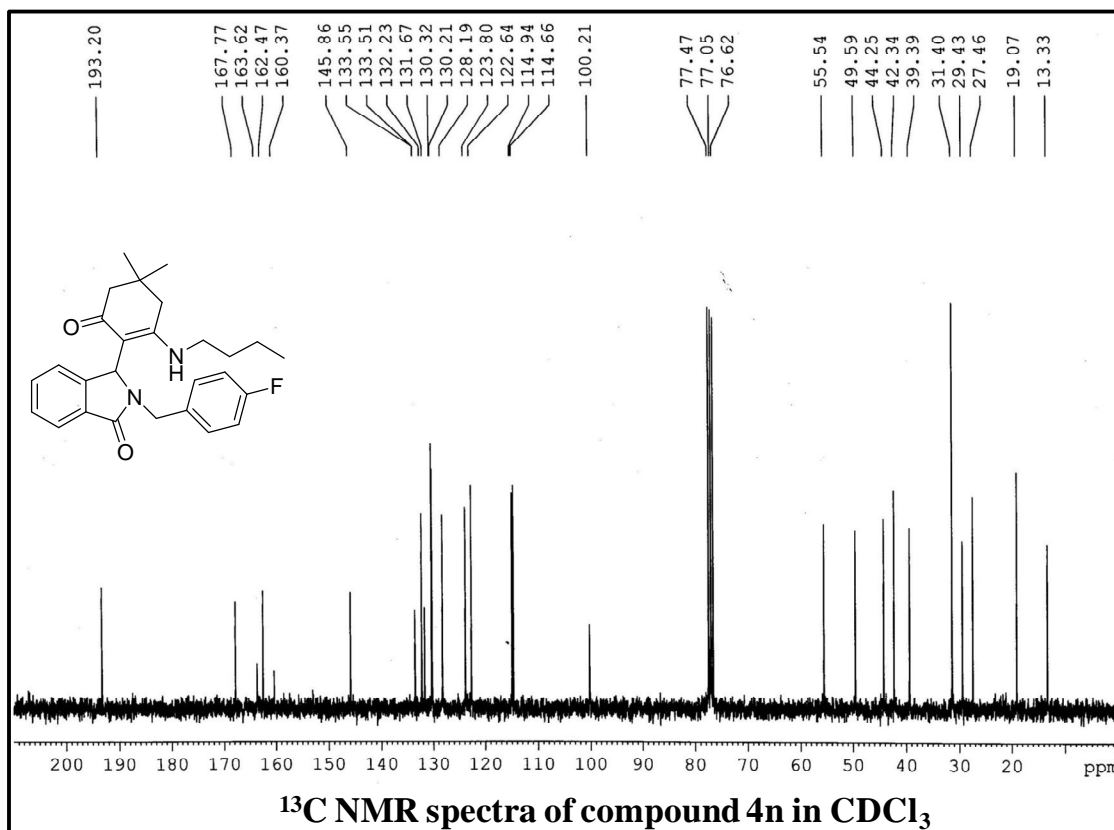
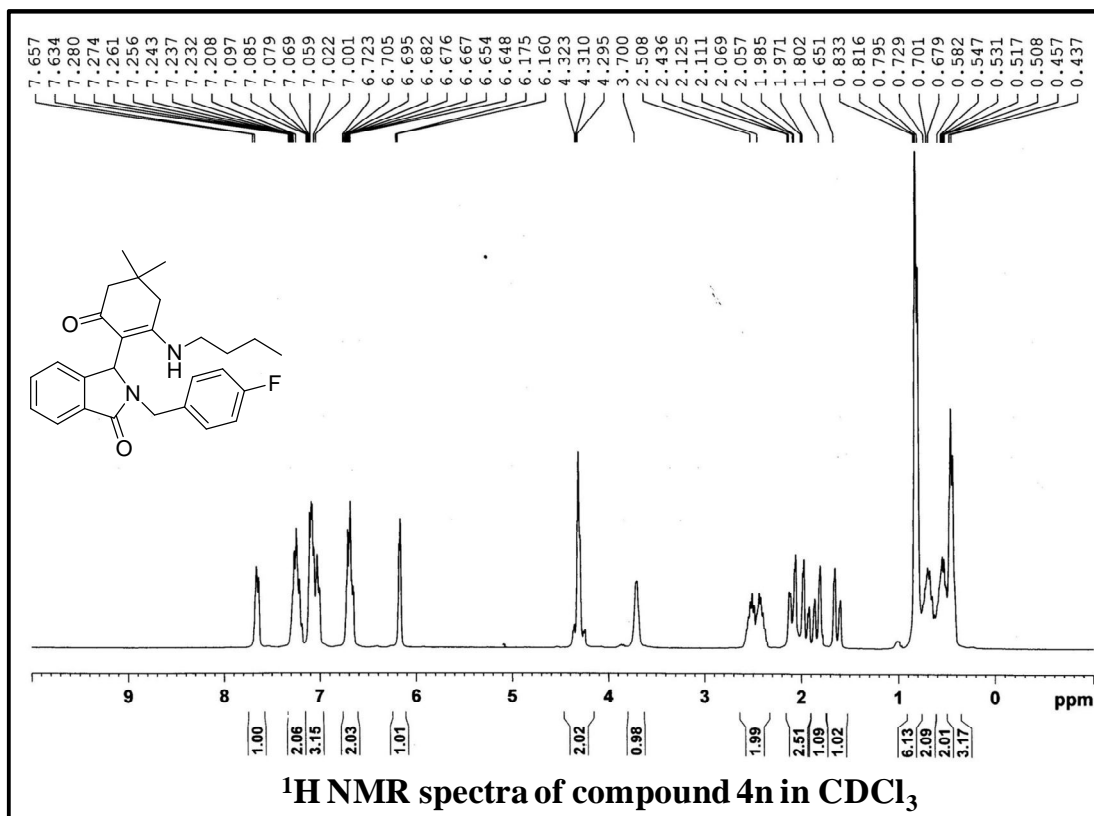


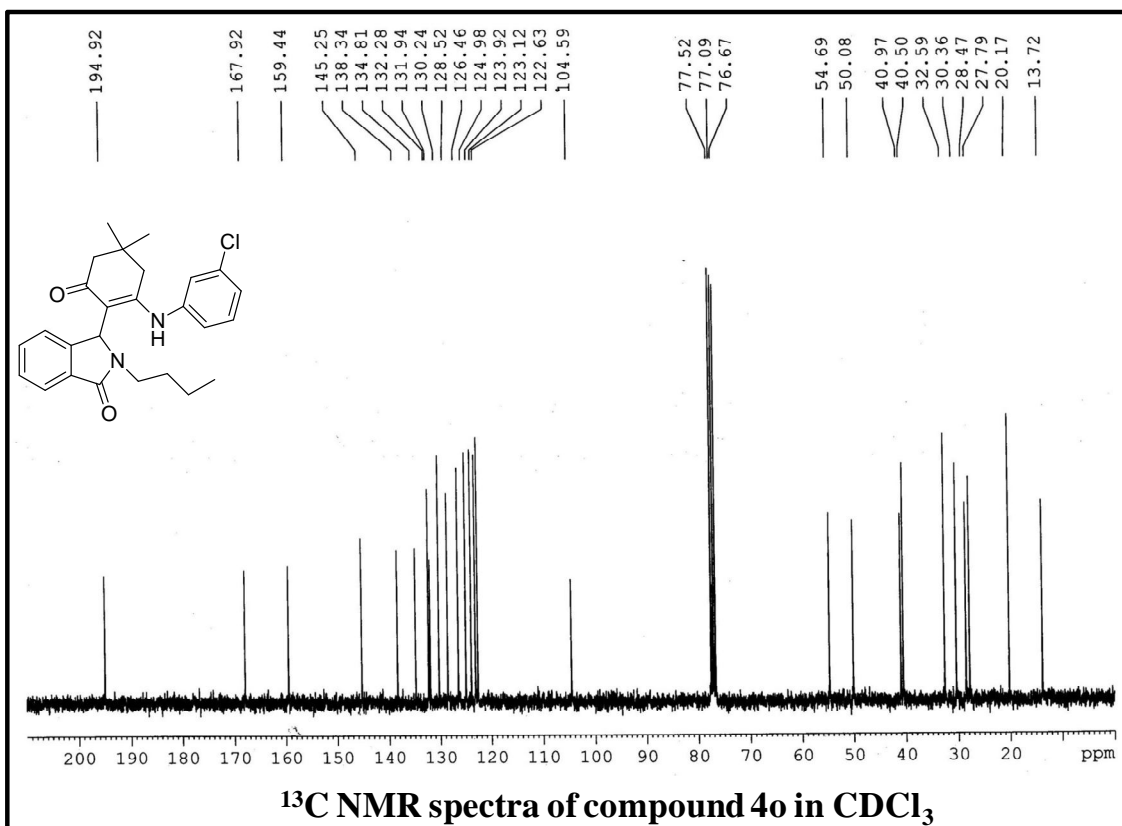
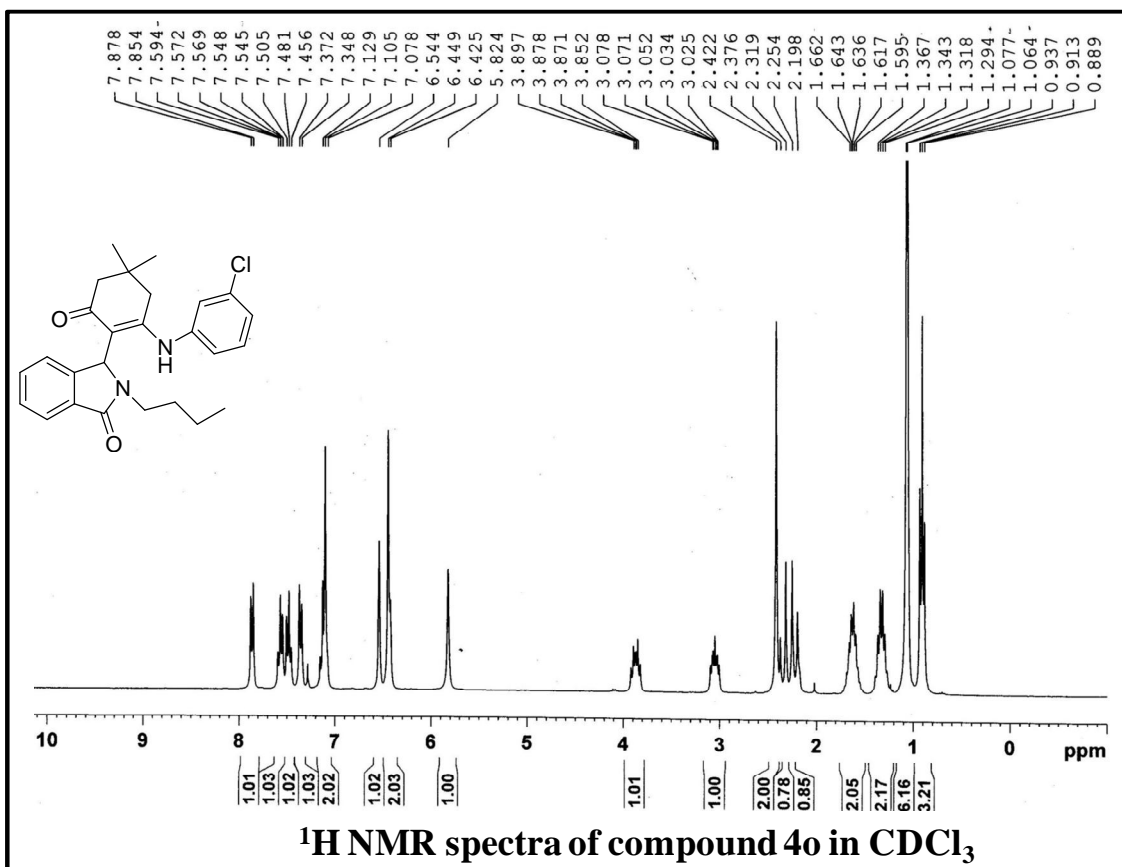


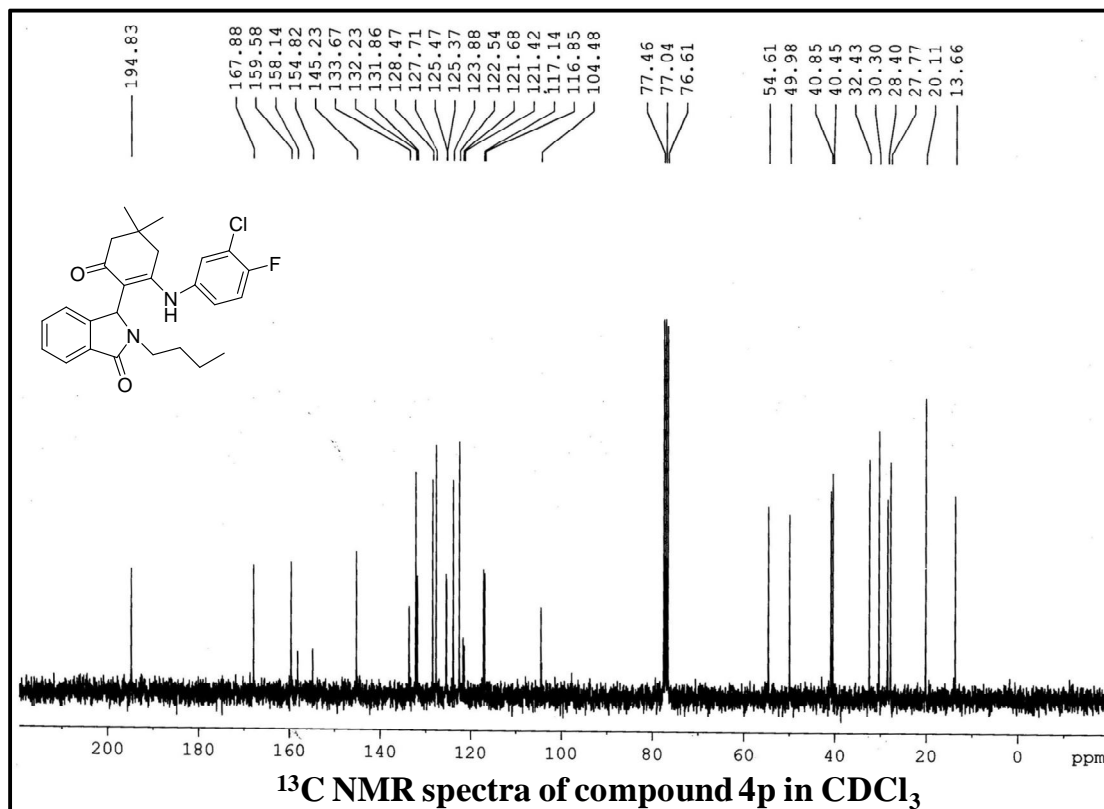
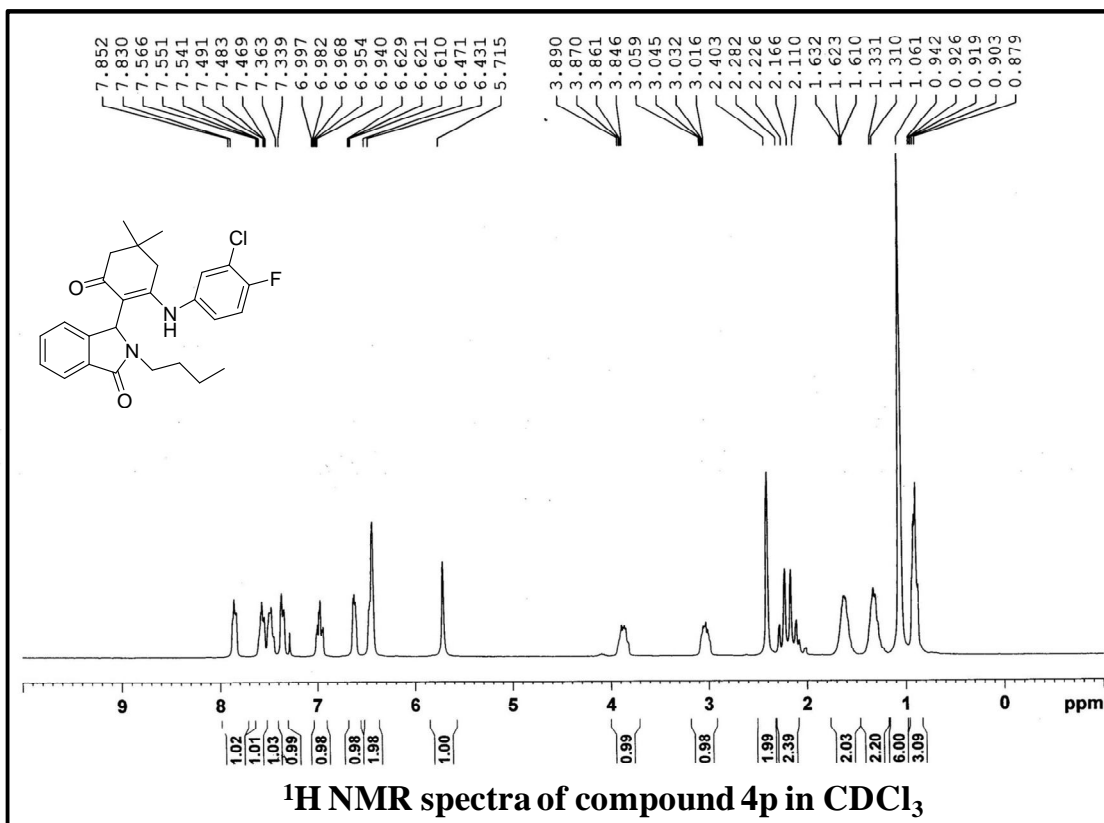


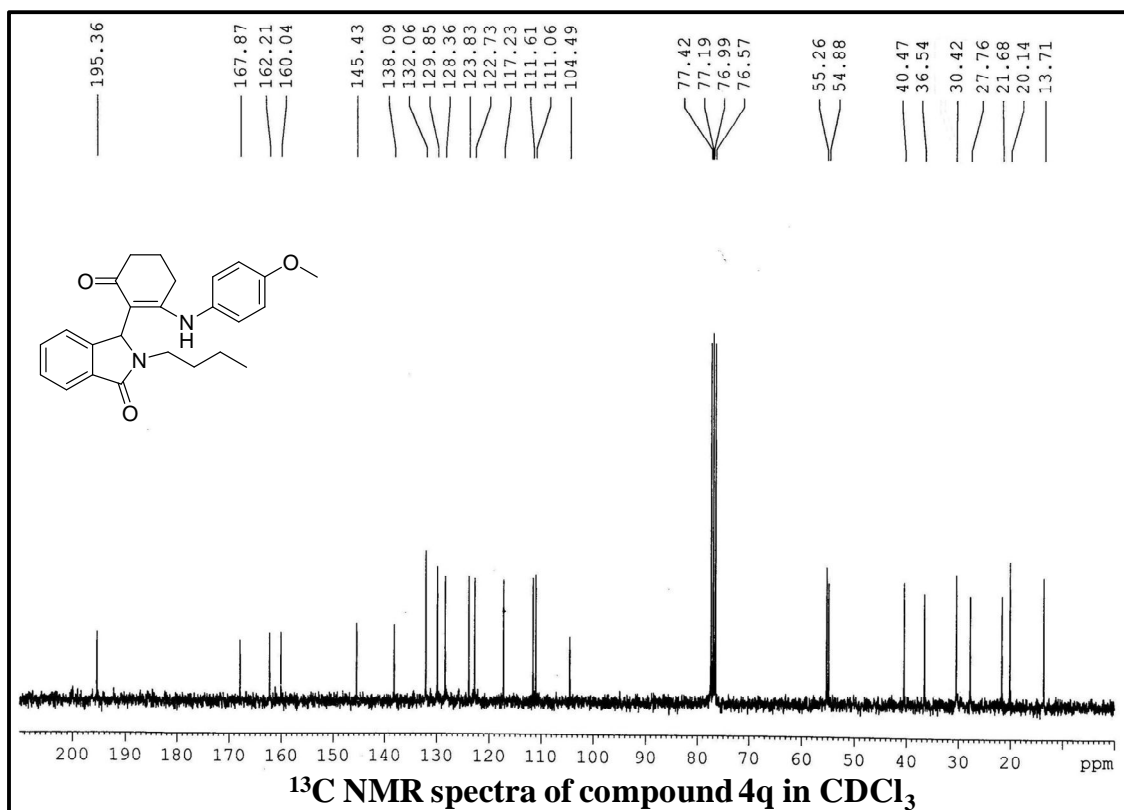
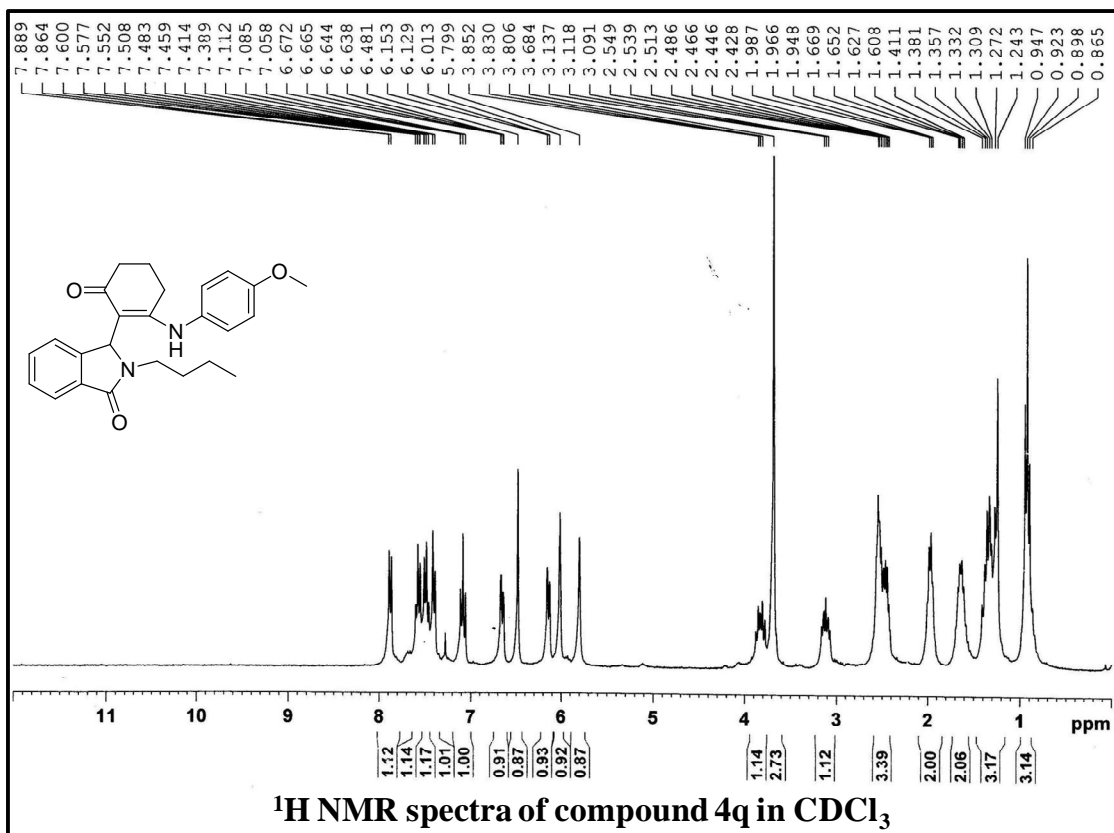


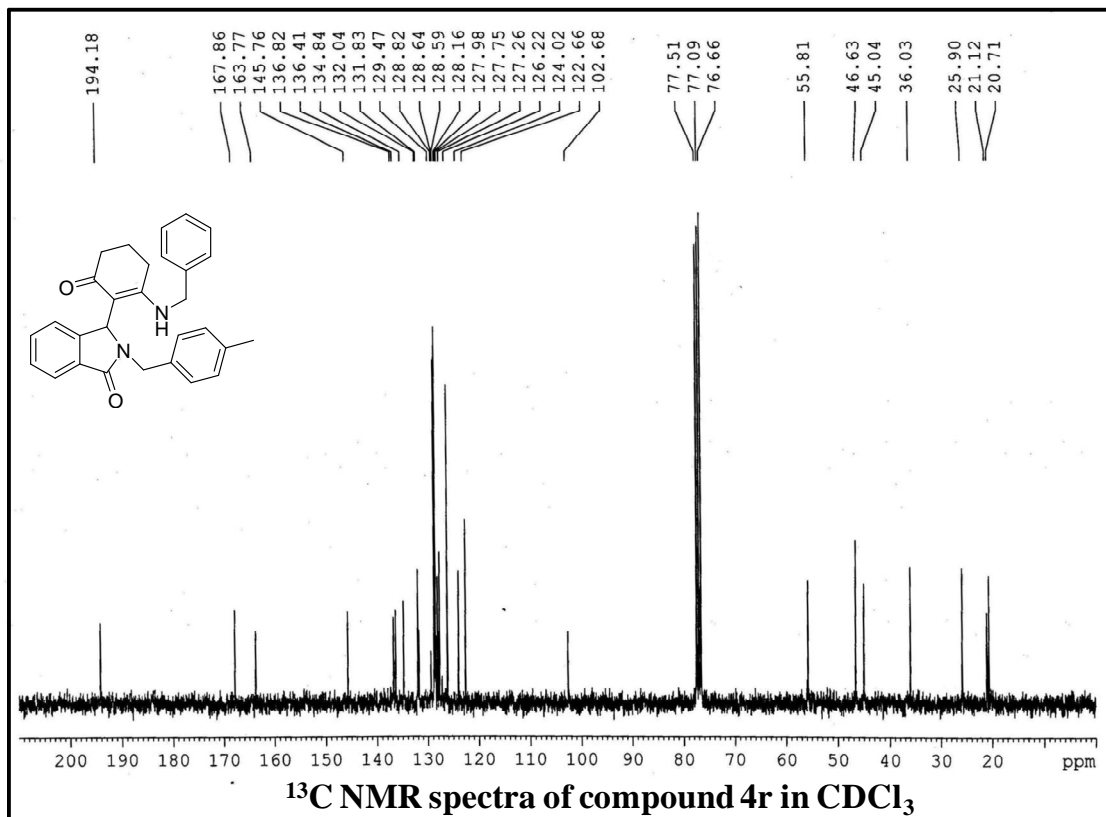
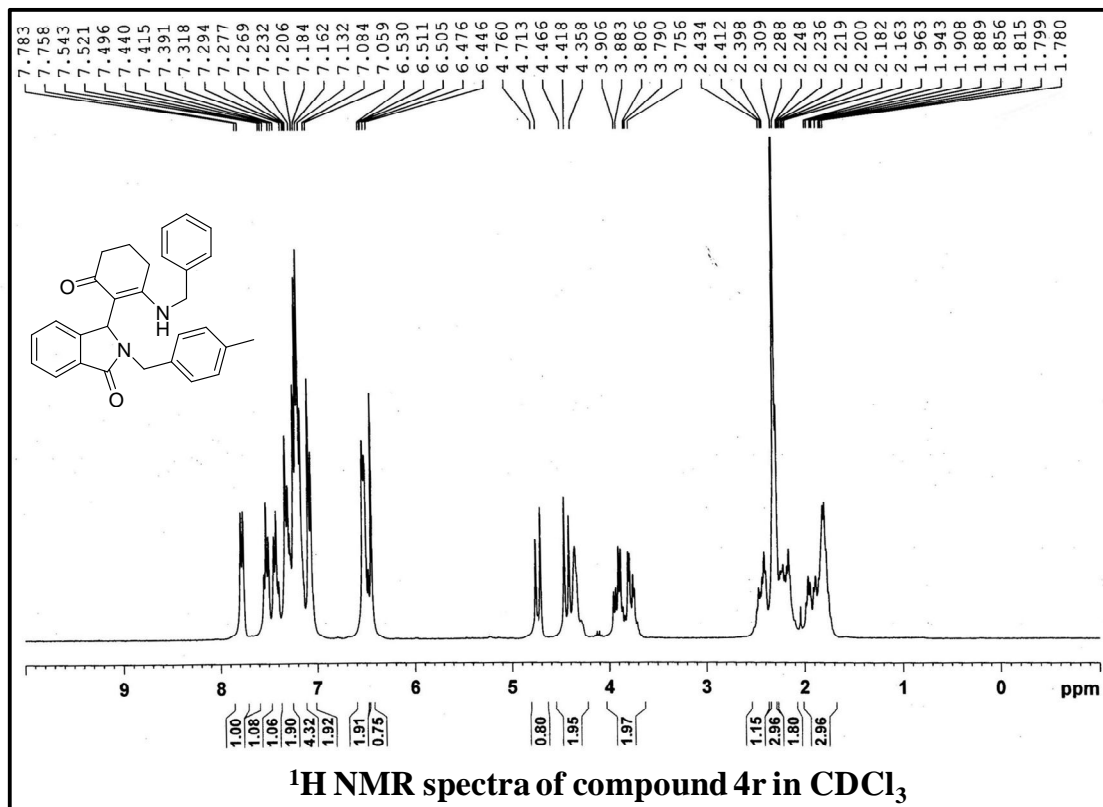


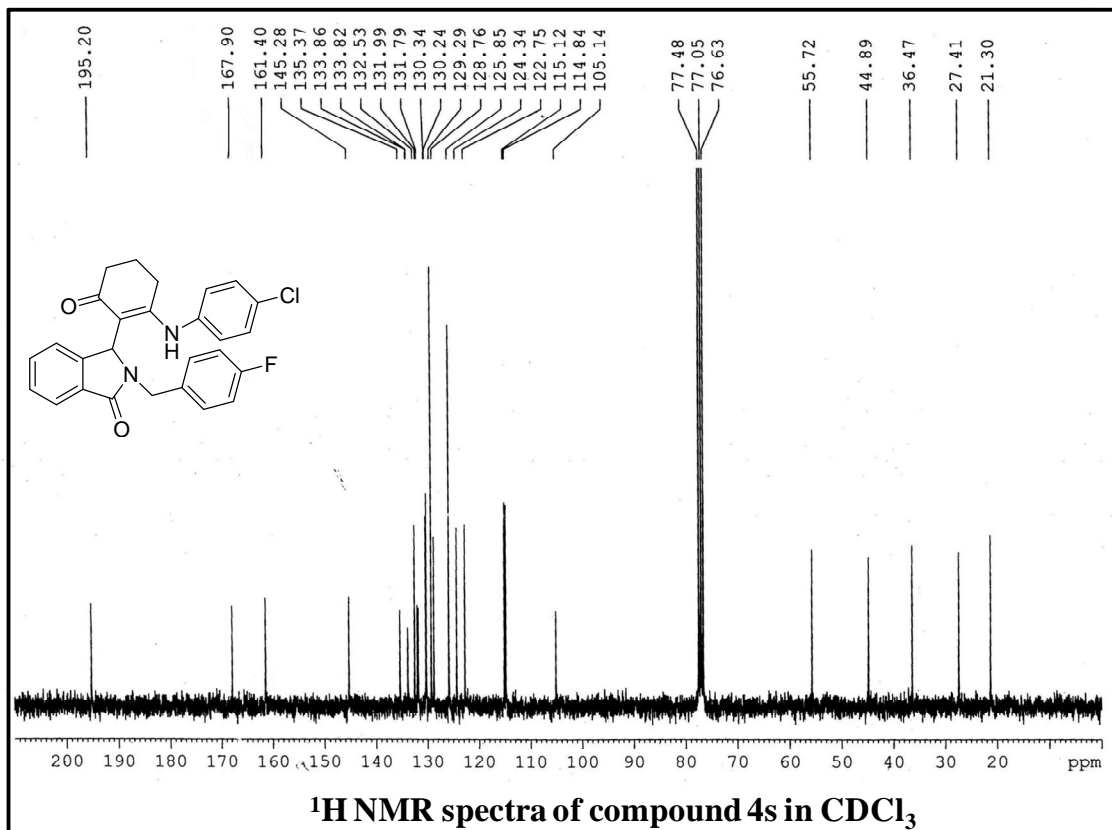
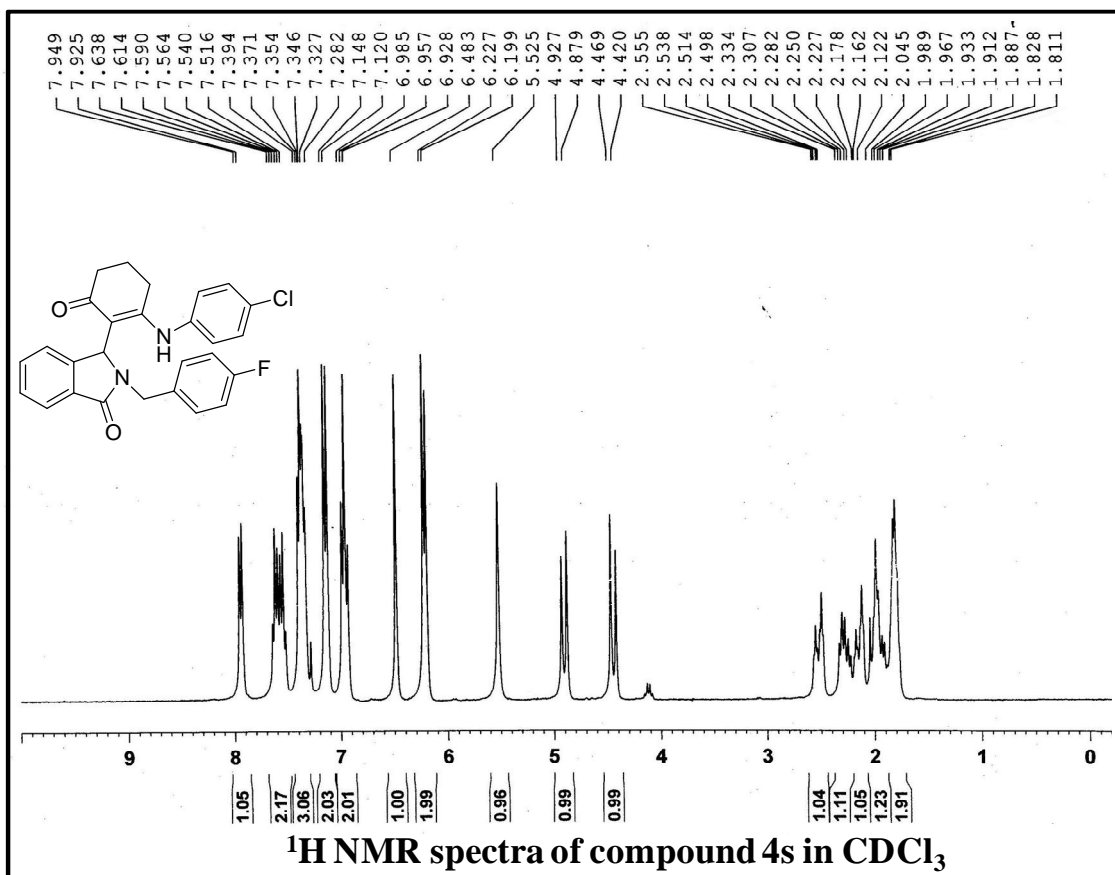


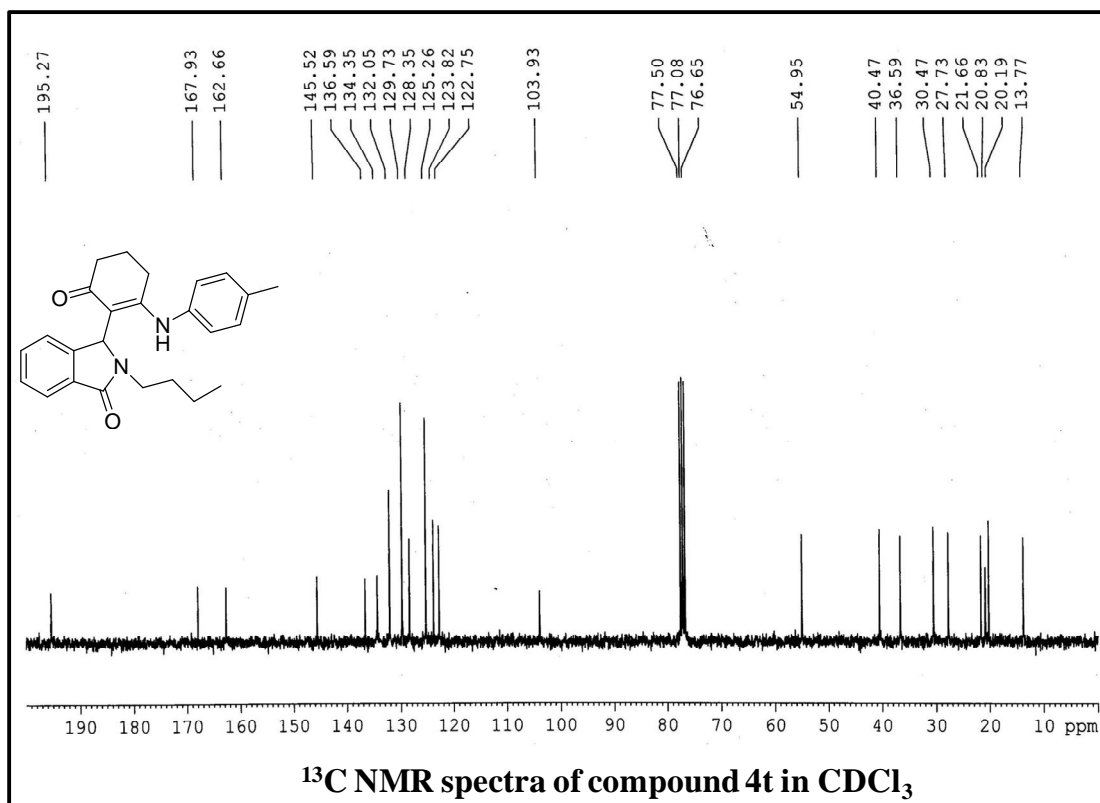
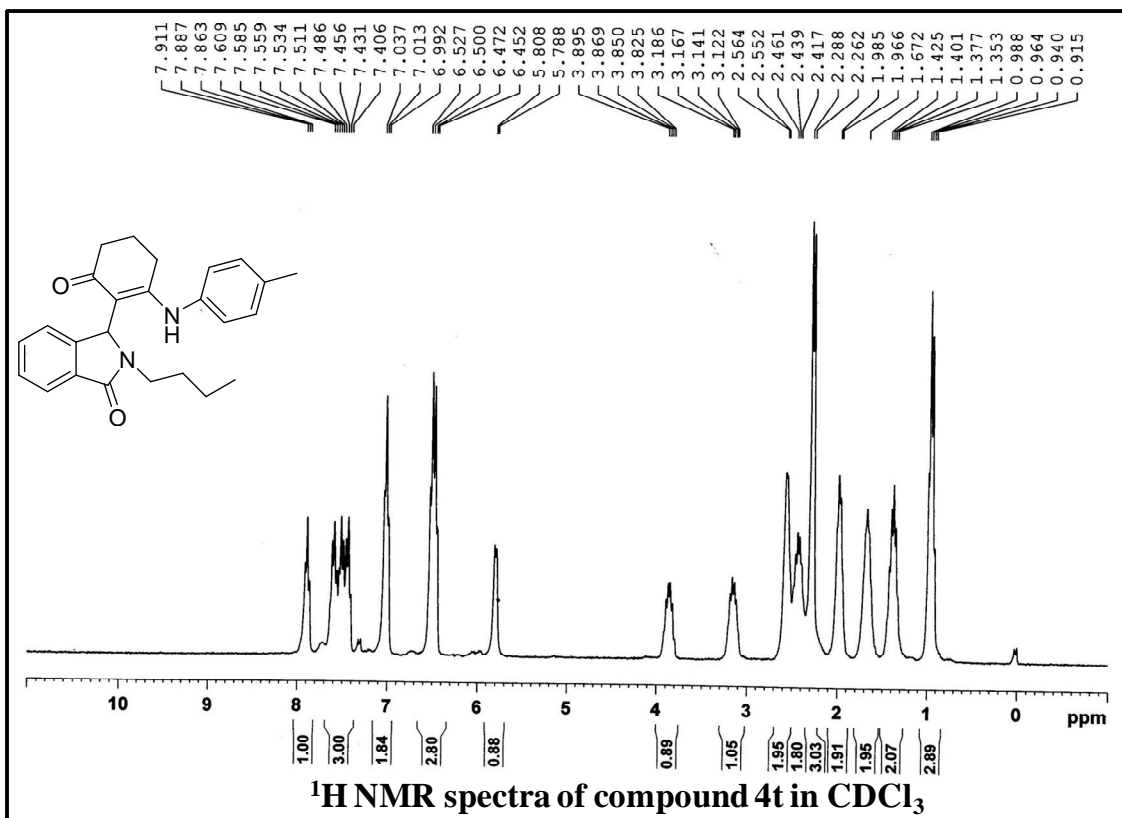


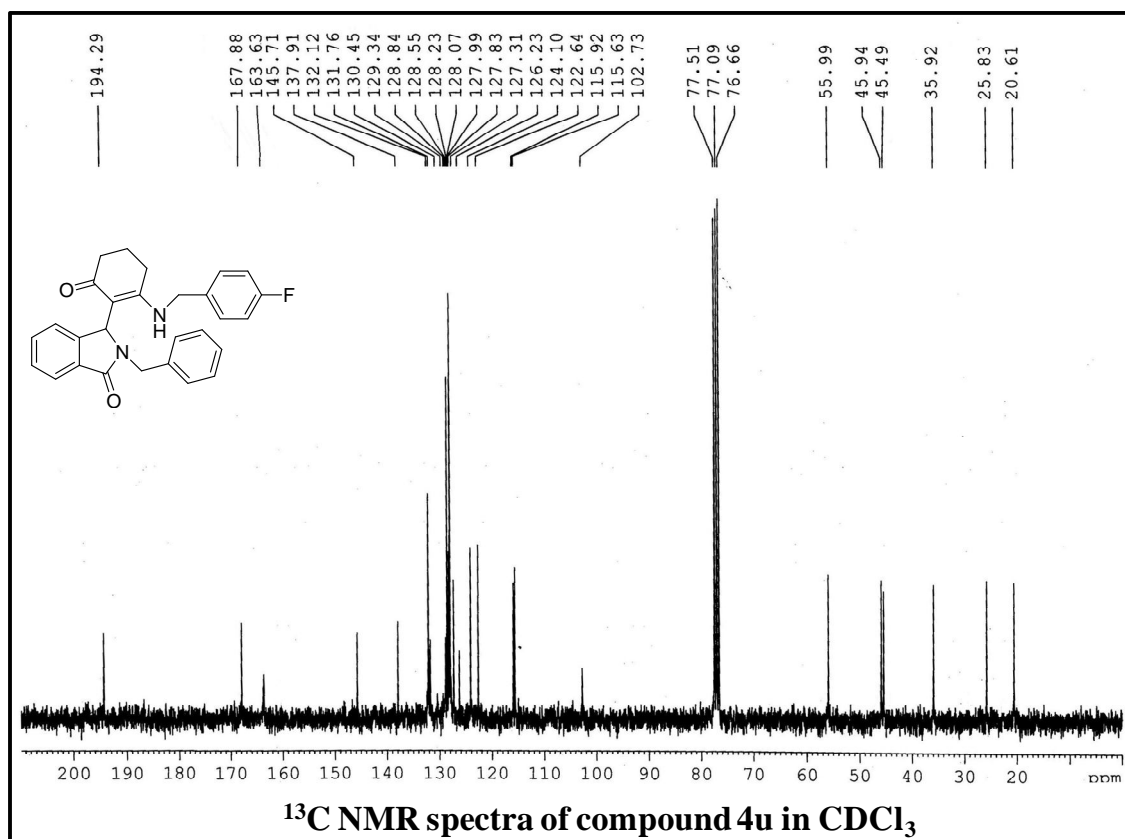
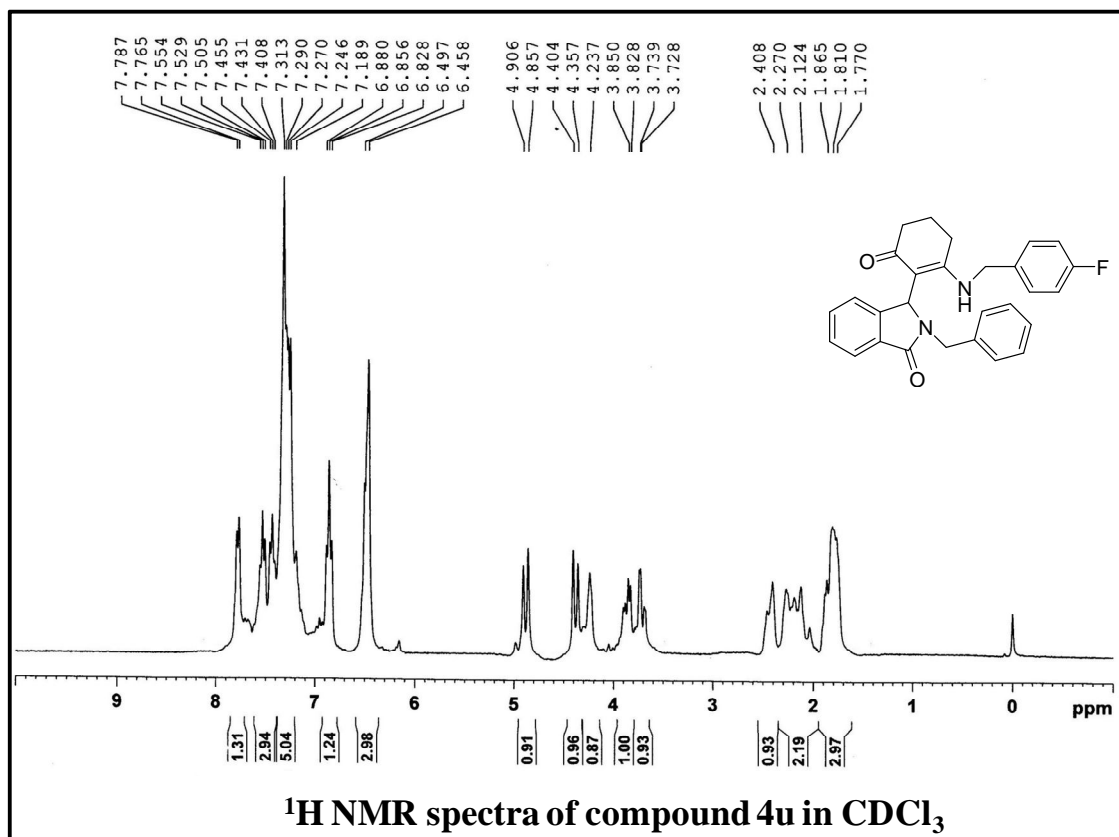












Reaction Scheme:

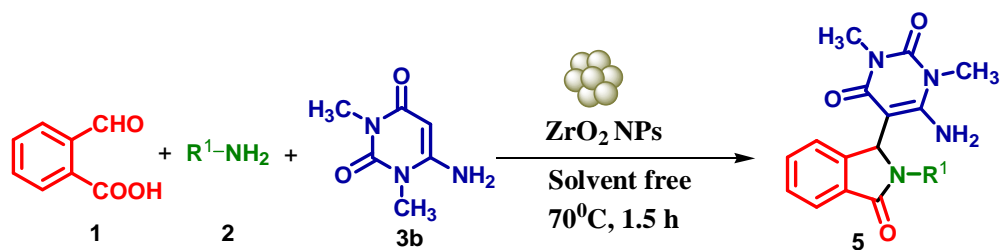
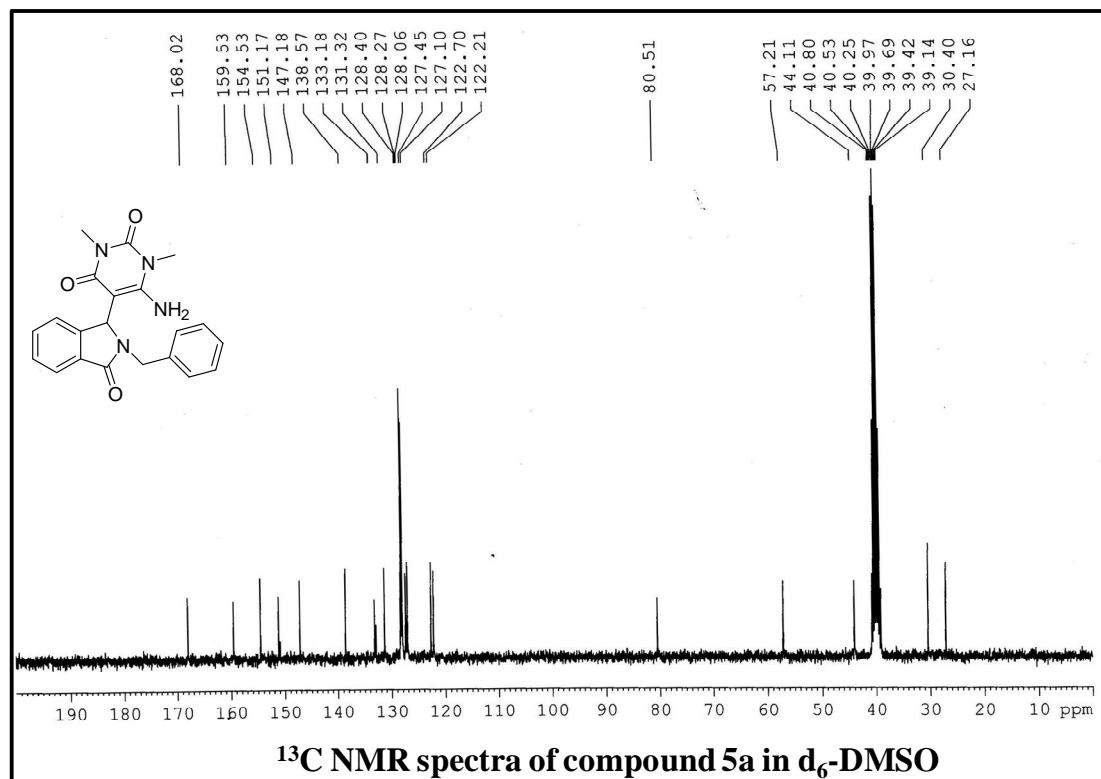
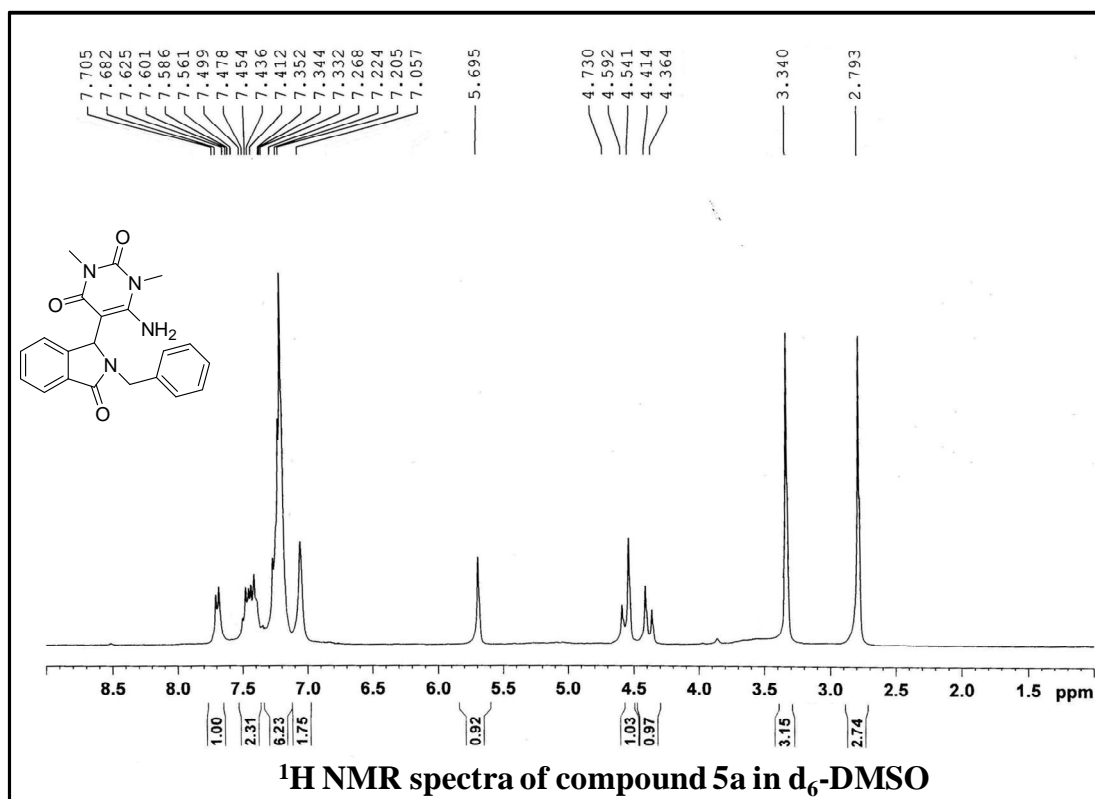


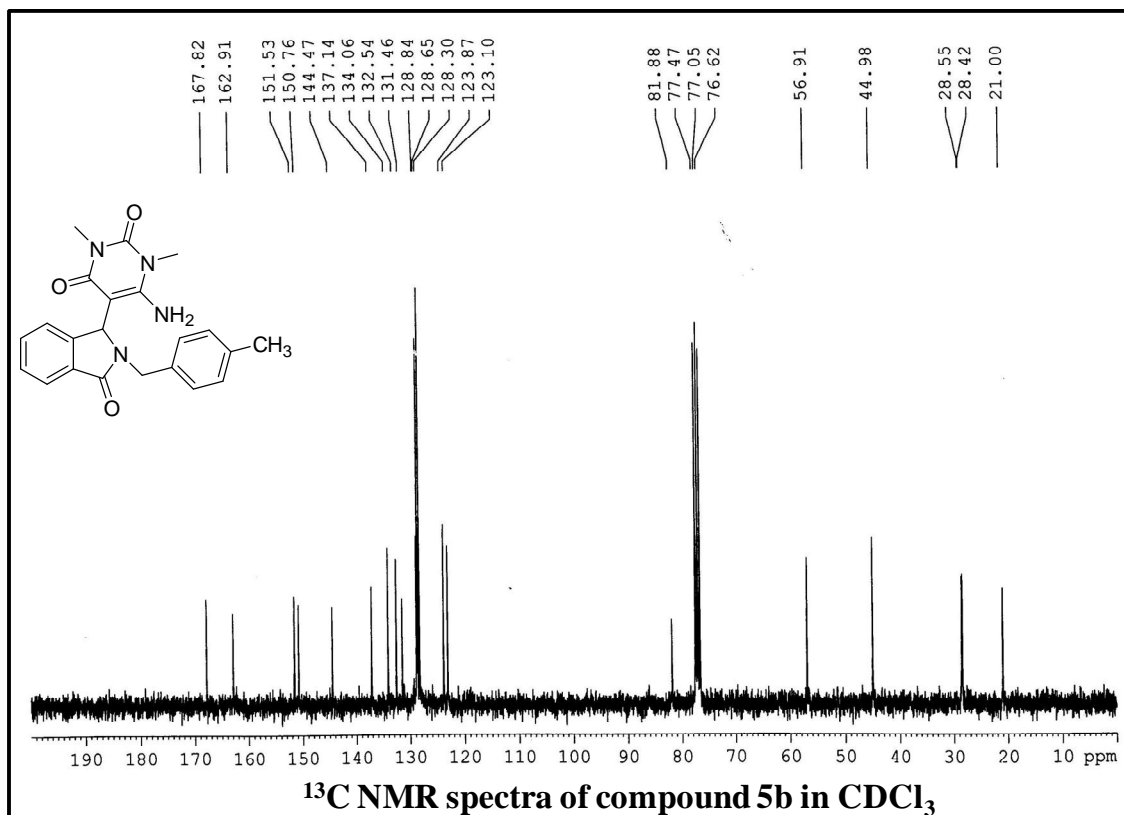
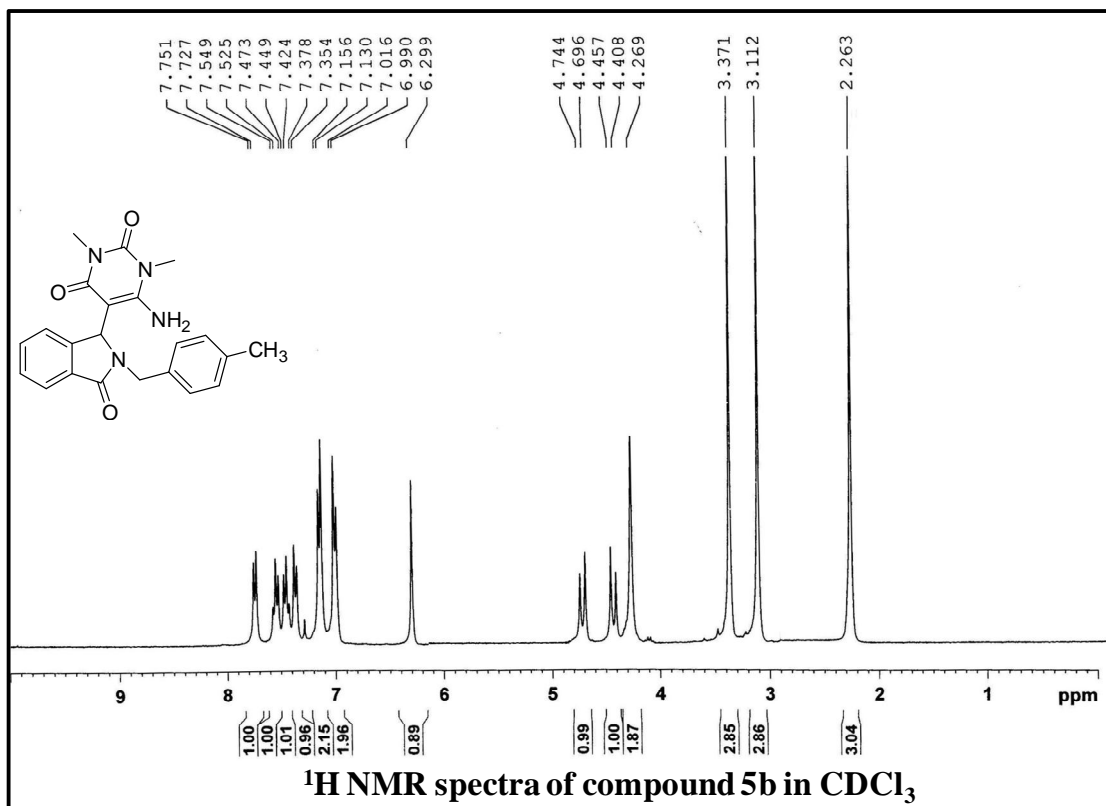
Table S2: Synthesis of isoindolin-1-ones **5a-d** through a three-component reaction

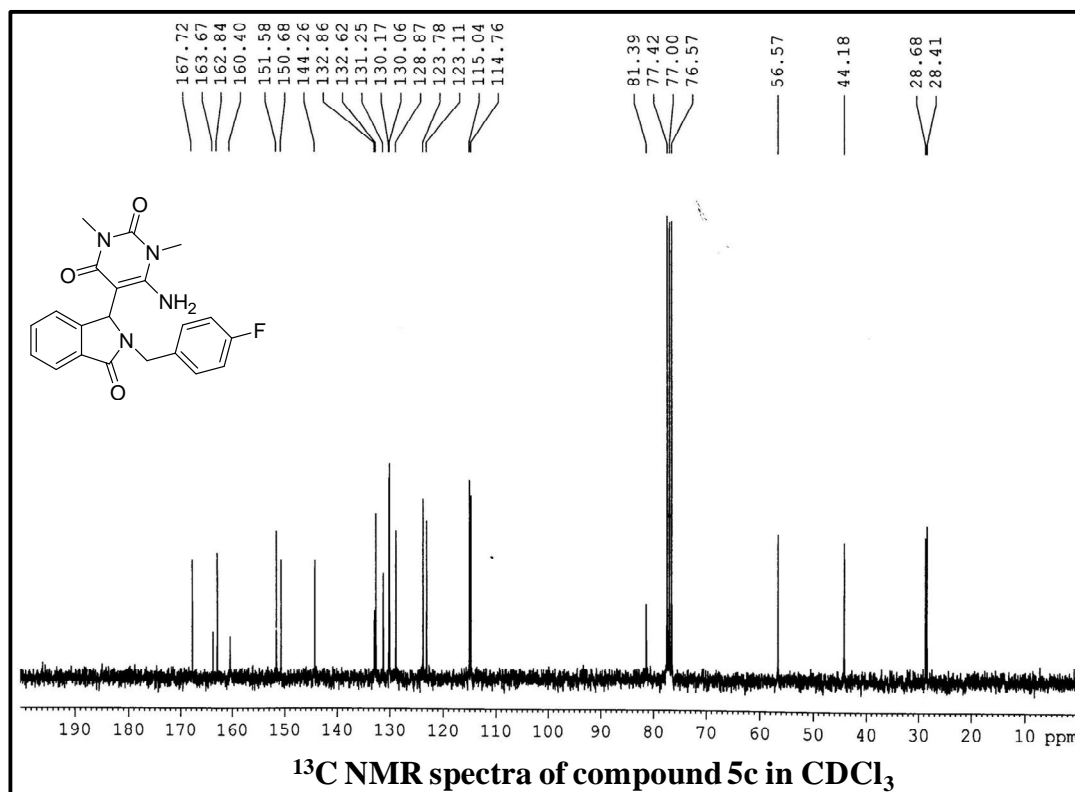
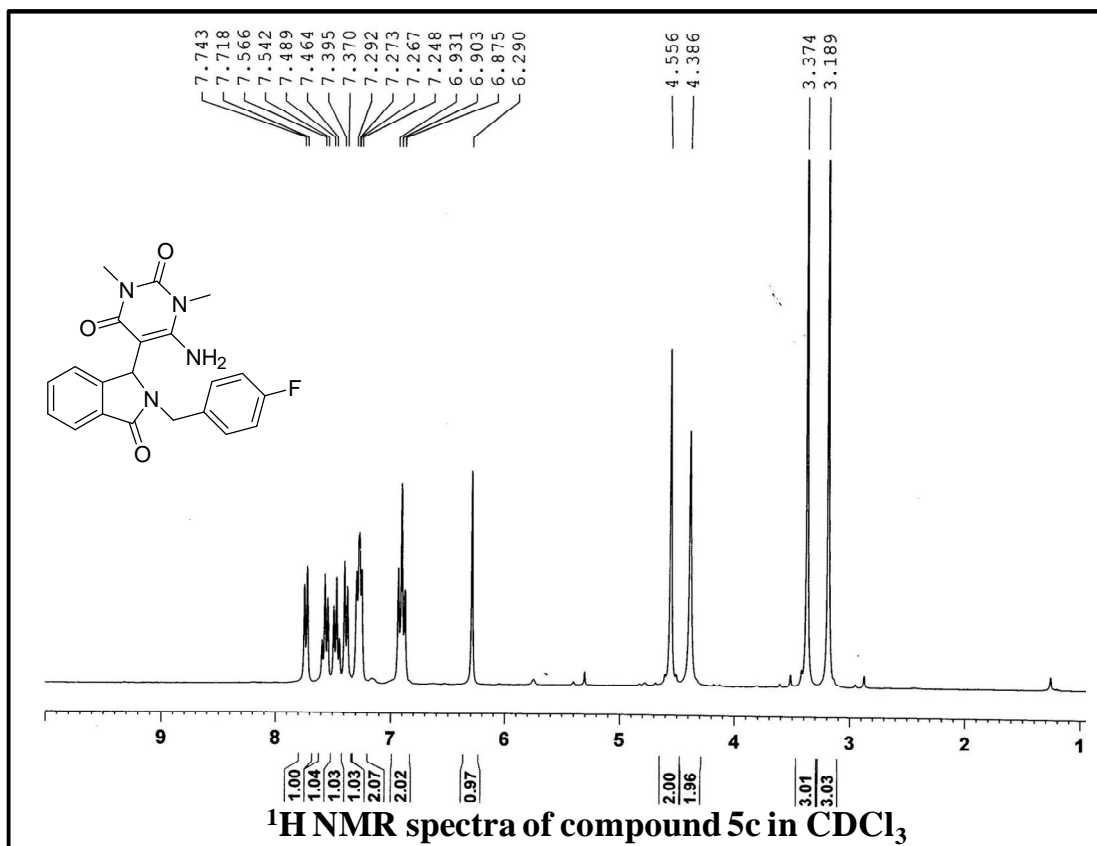
Entry	1	2	3a	4	Yield (%) ^a	Melting Point ($^\circ\text{C}$)
1					85	200-202
2					88	142-144
3					80	180-182
4					83	160-162

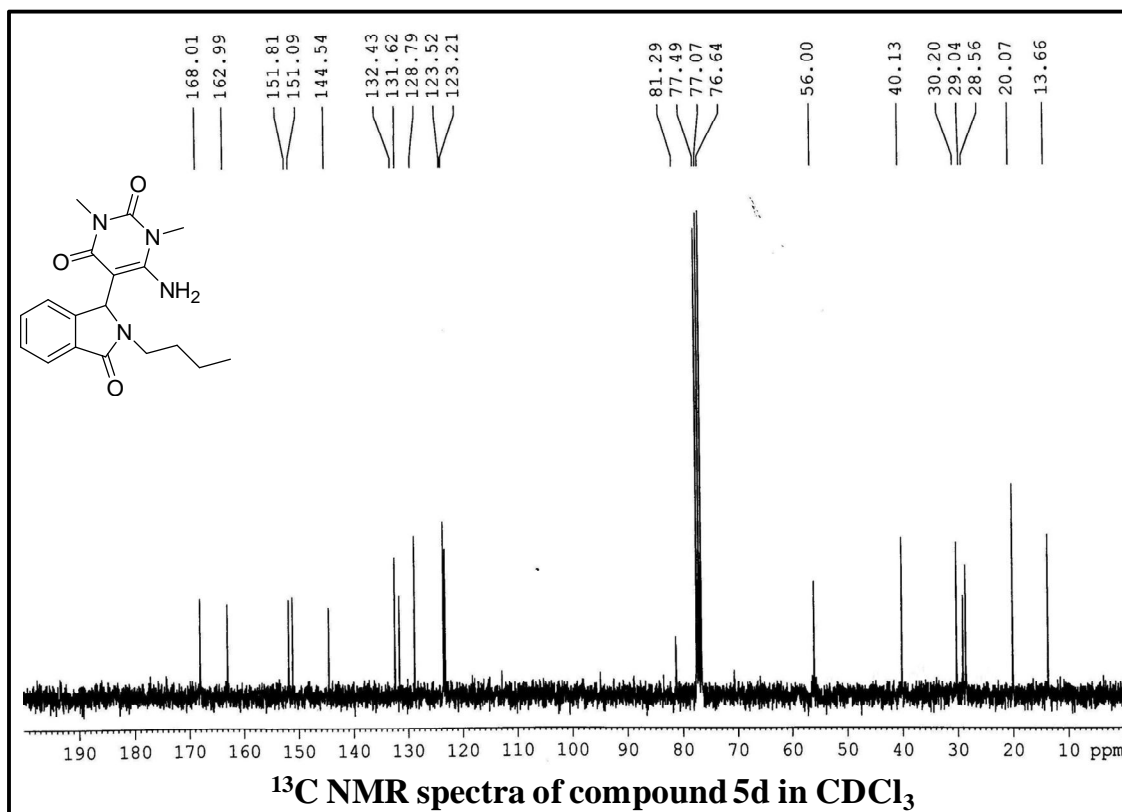
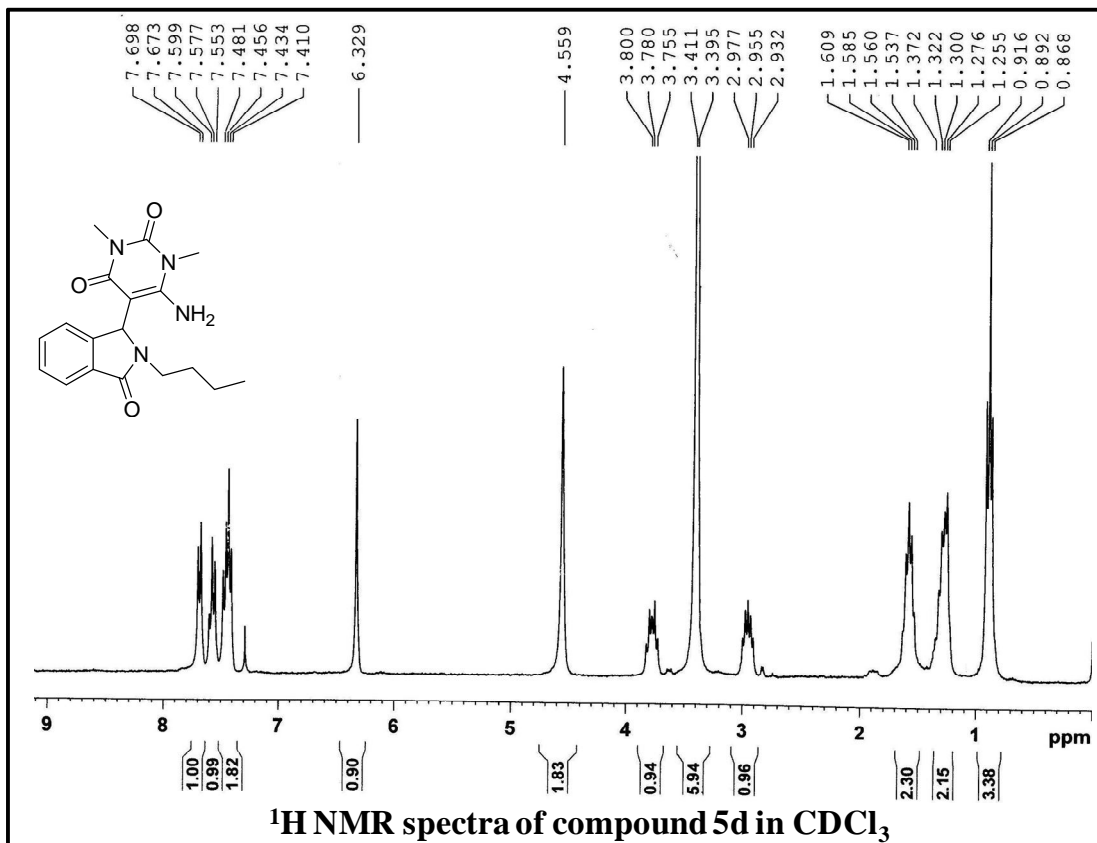
^aIsolated Yields (%)

Spectral Data 5a-d:









Reaction Scheme:

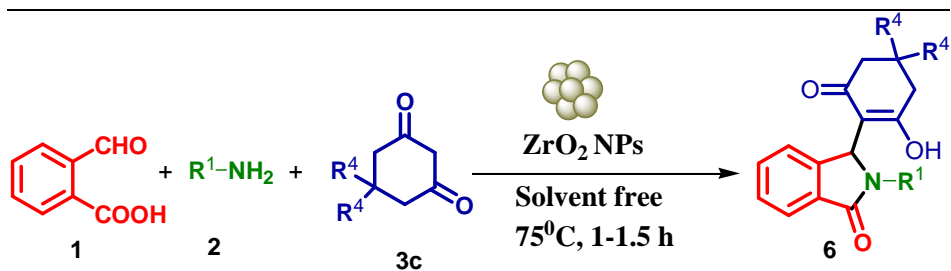
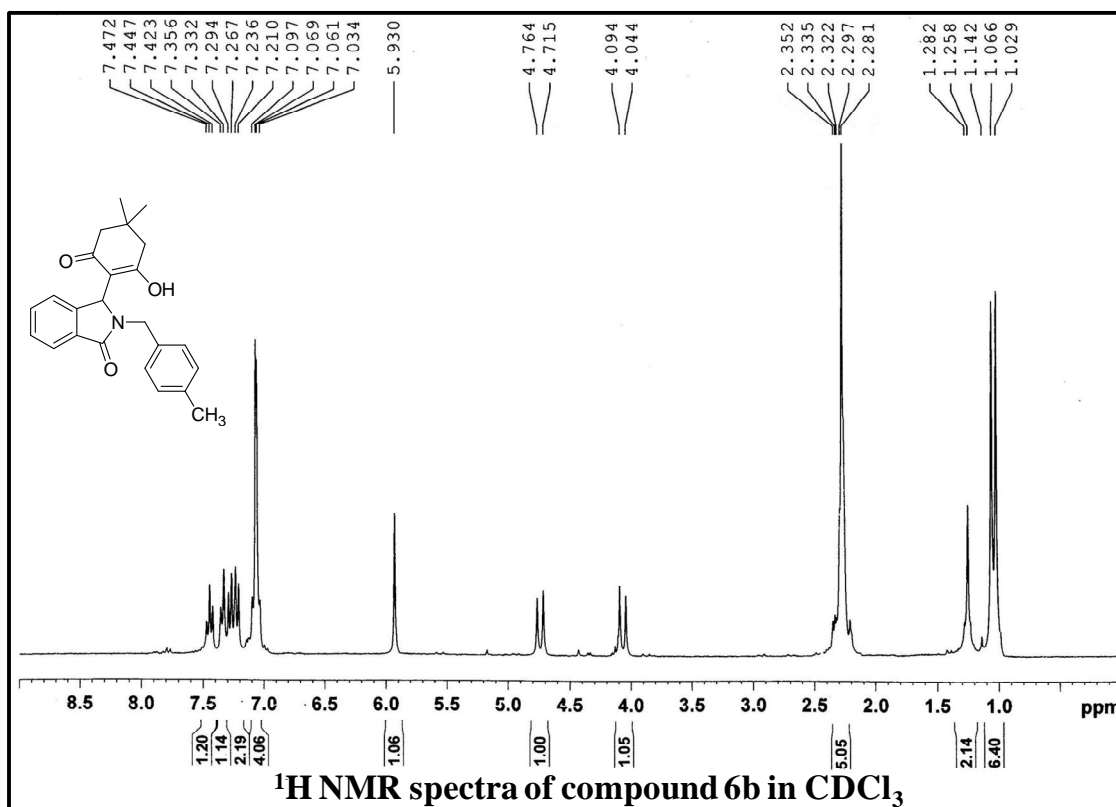
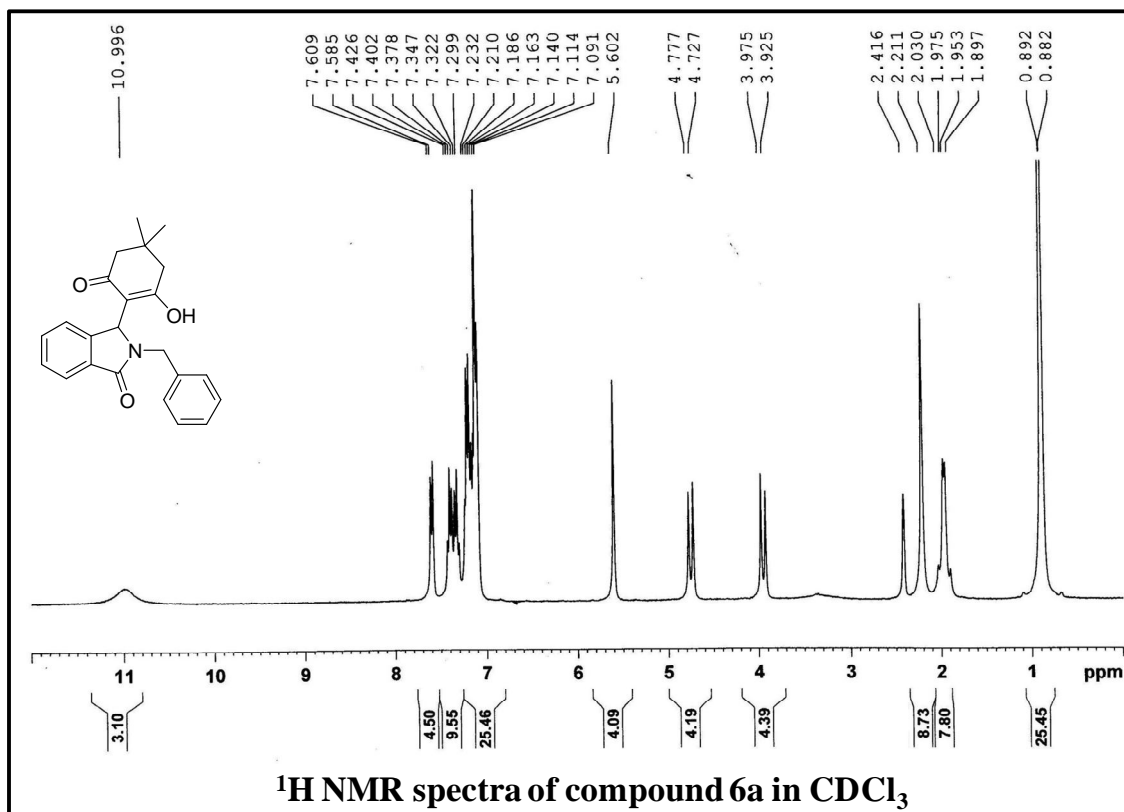


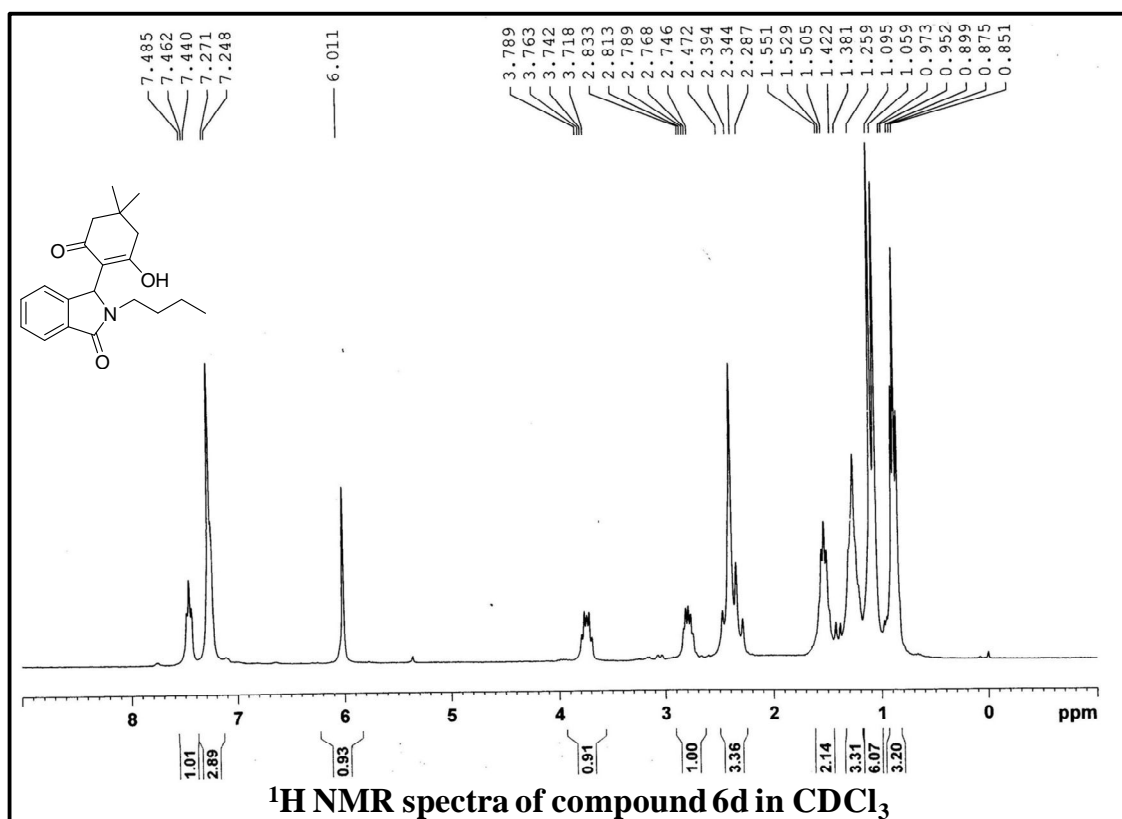
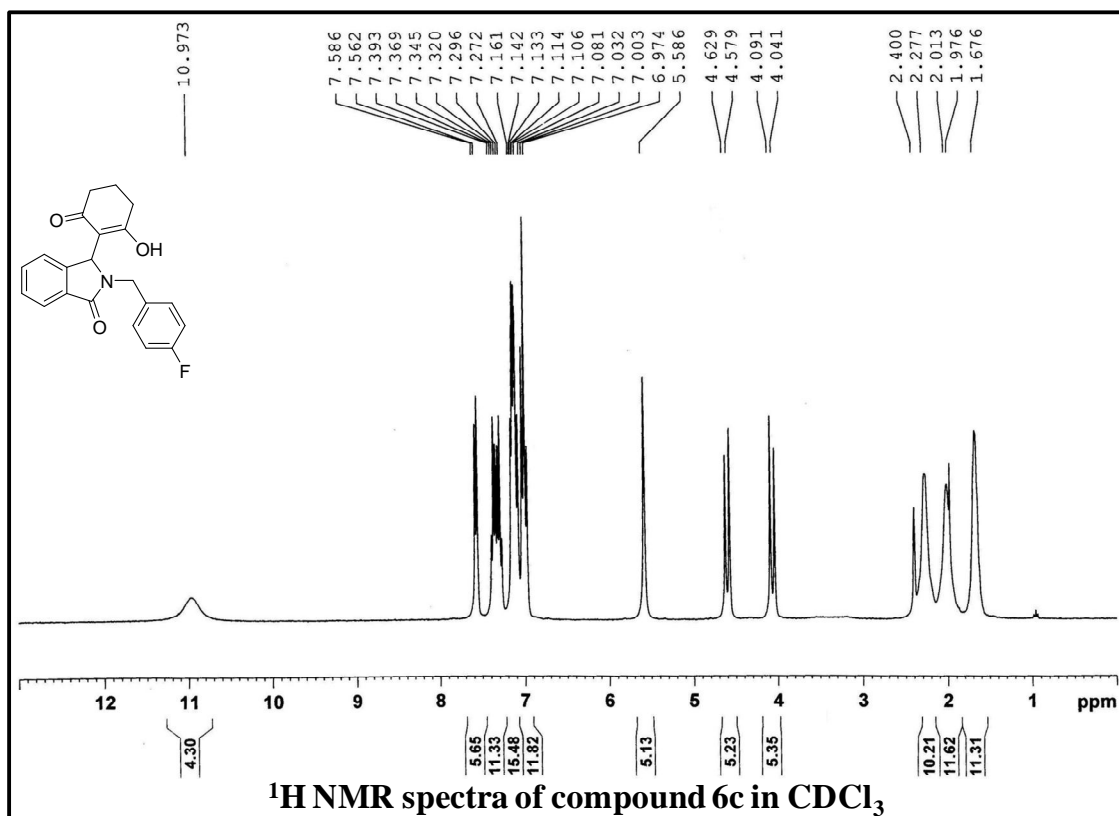
Table S3: Synthesis of isoindolin-1-ones **6a-d** through a three-component reaction

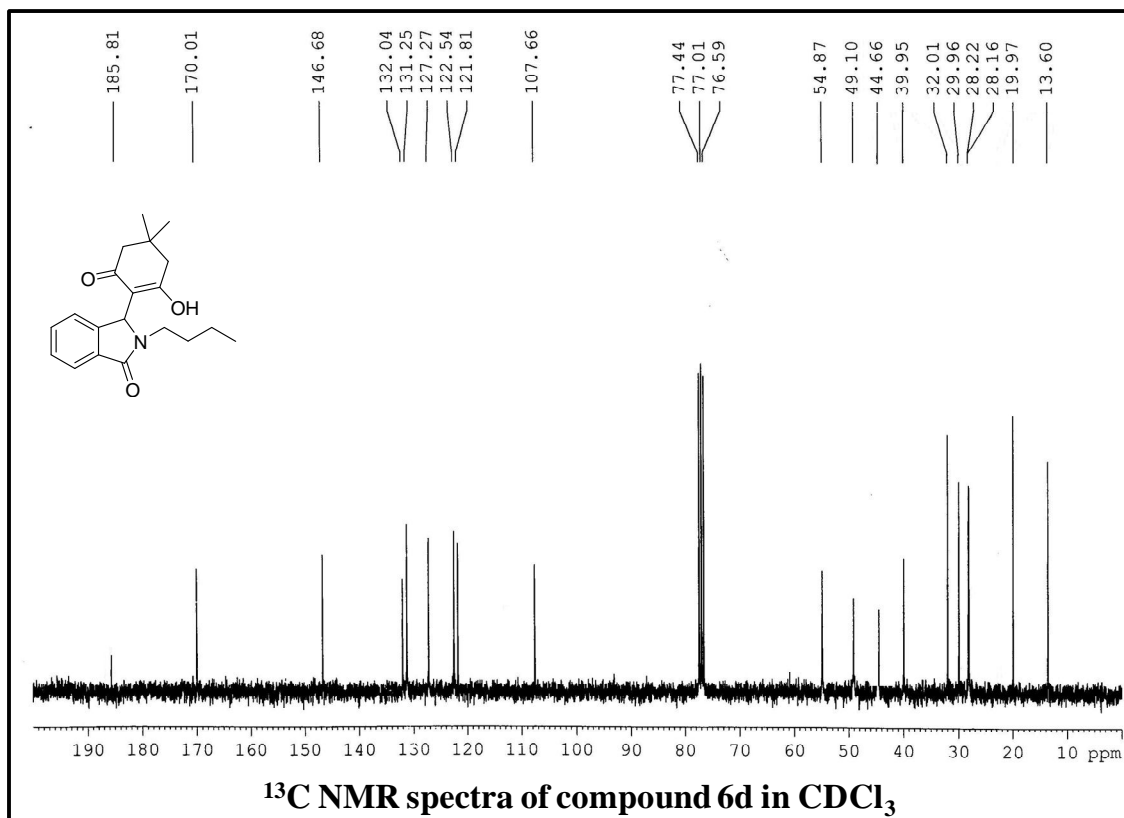
Entry	1	2	3c	6	Yield (%) ^a	Literature m.p [1]/ Observed m.p (°C)
1					95	220 / 216-218
2					92	247 / 242-244
3					90	229 / 230-232
4					87	226-228

^aIsolated Yield(%)

Spectral data 6a-d:







Reaction Scheme:

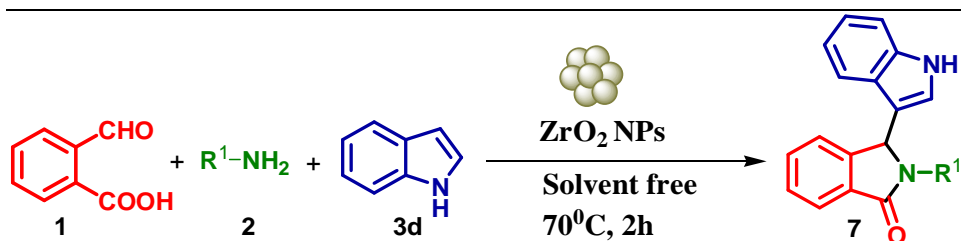
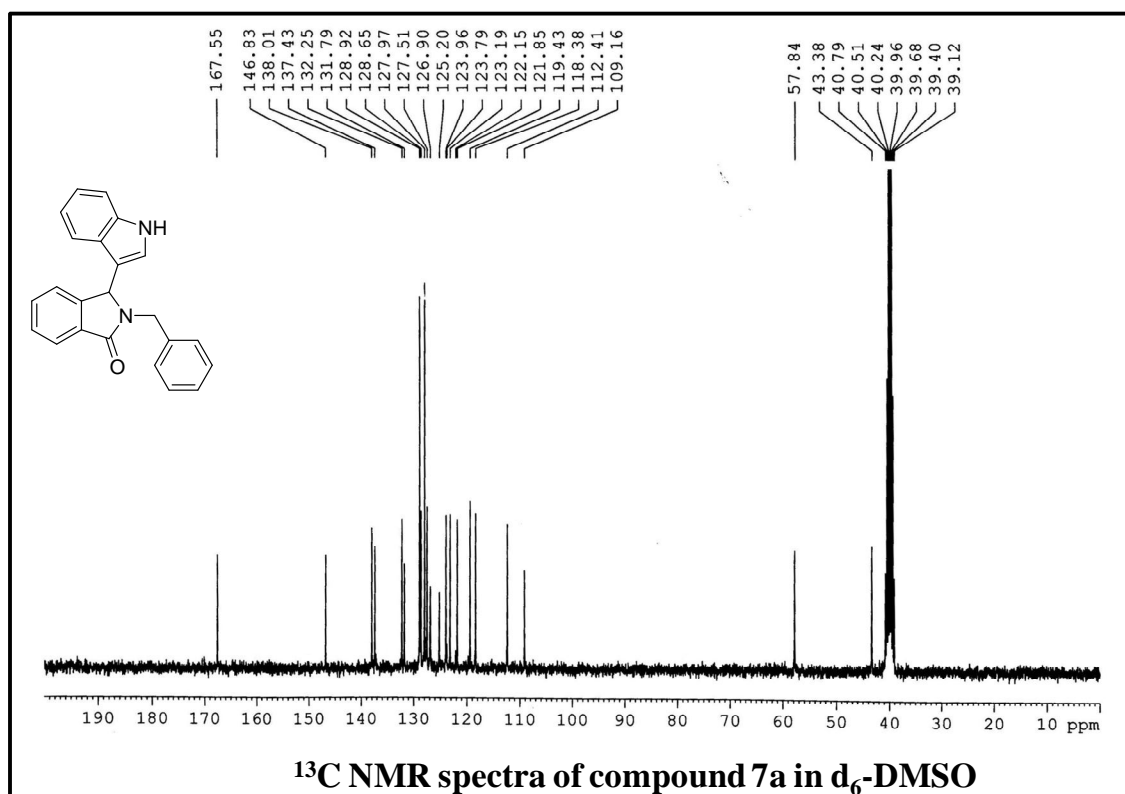
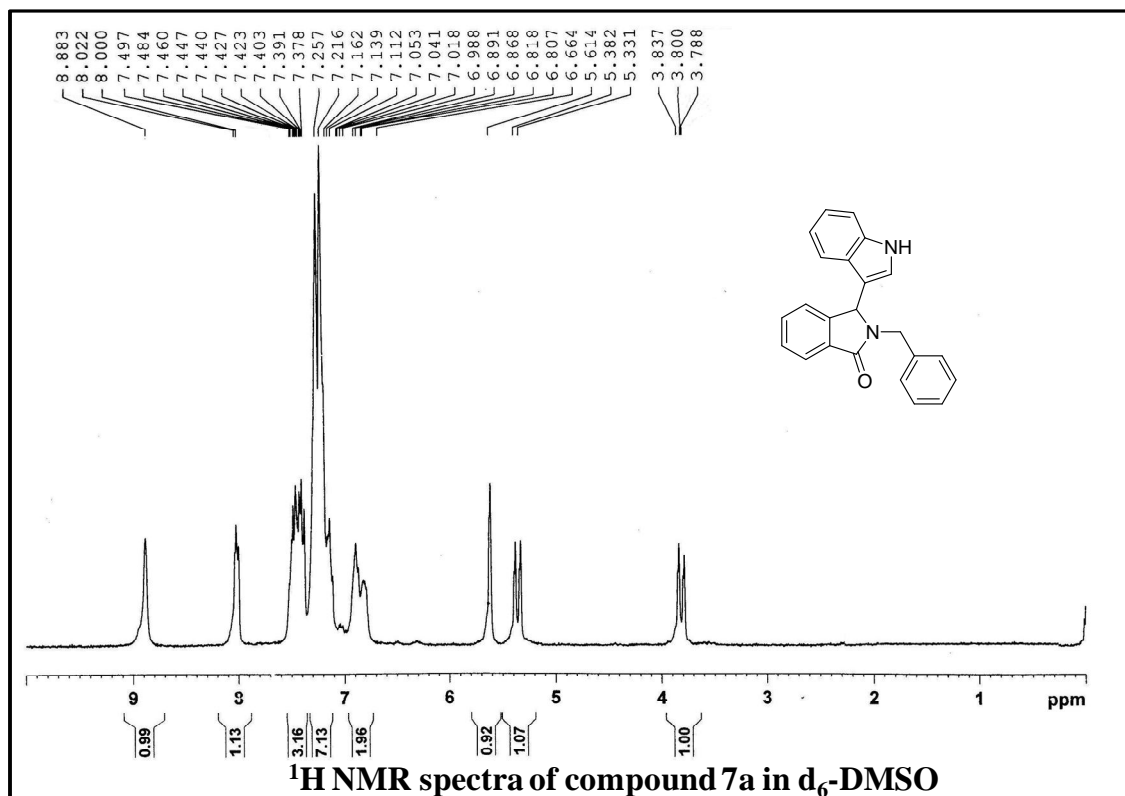


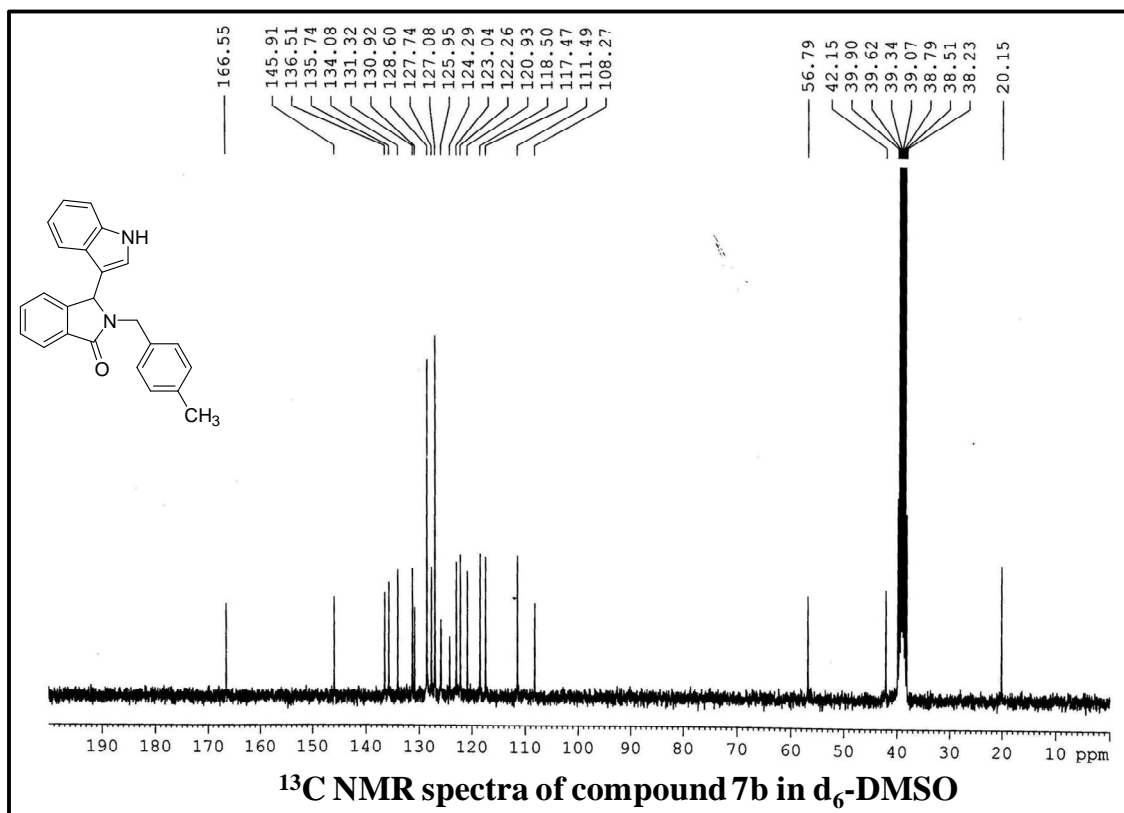
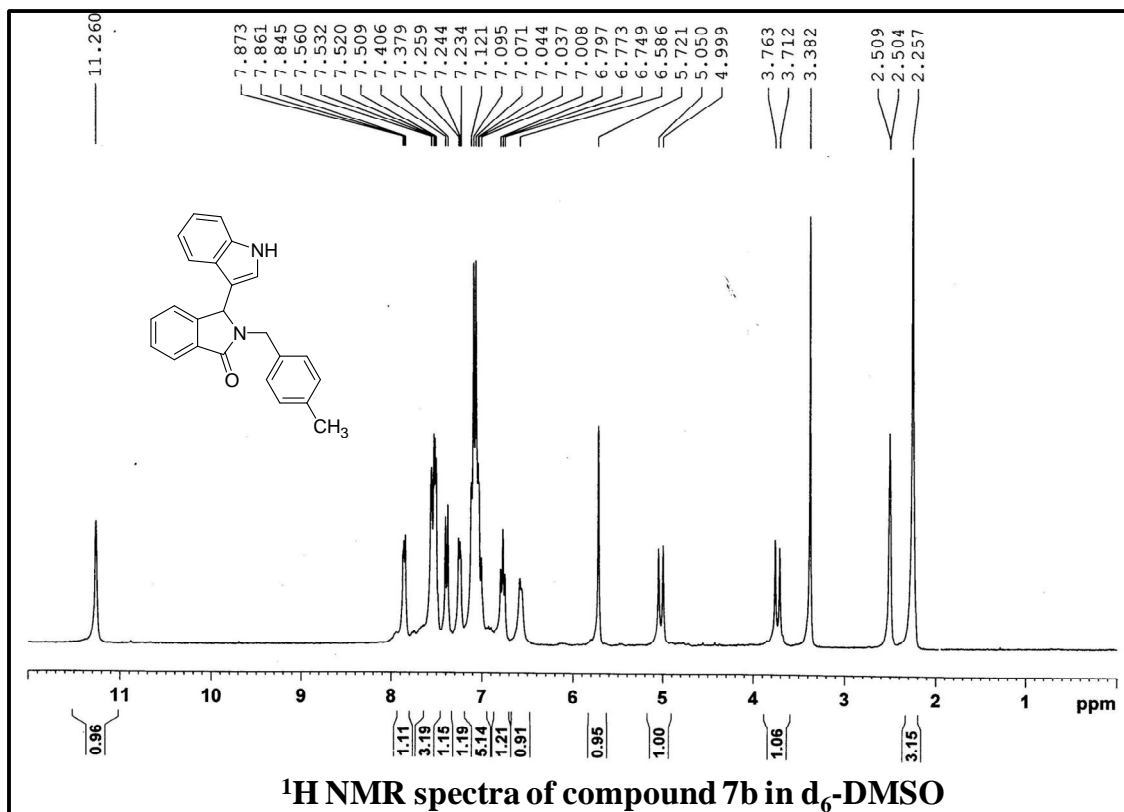
Table S4: Synthesis of isoindolin-1-ones **7a-d** through a three-component reaction

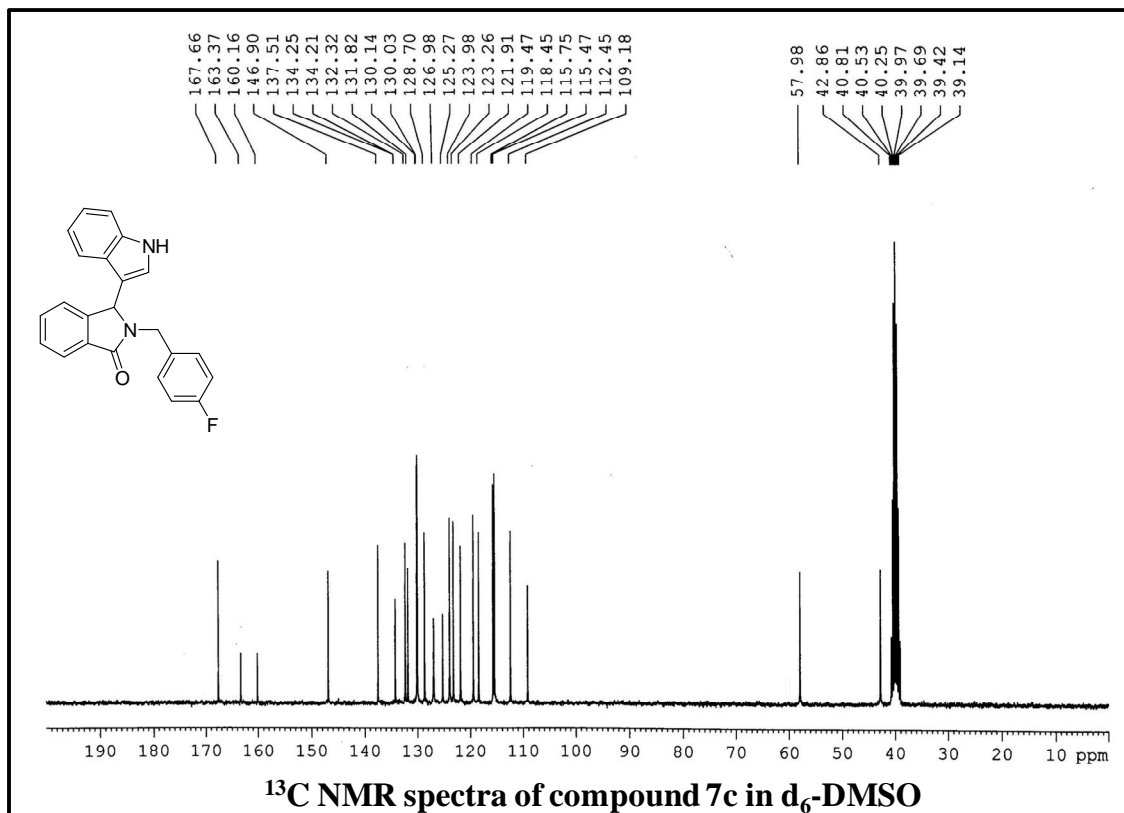
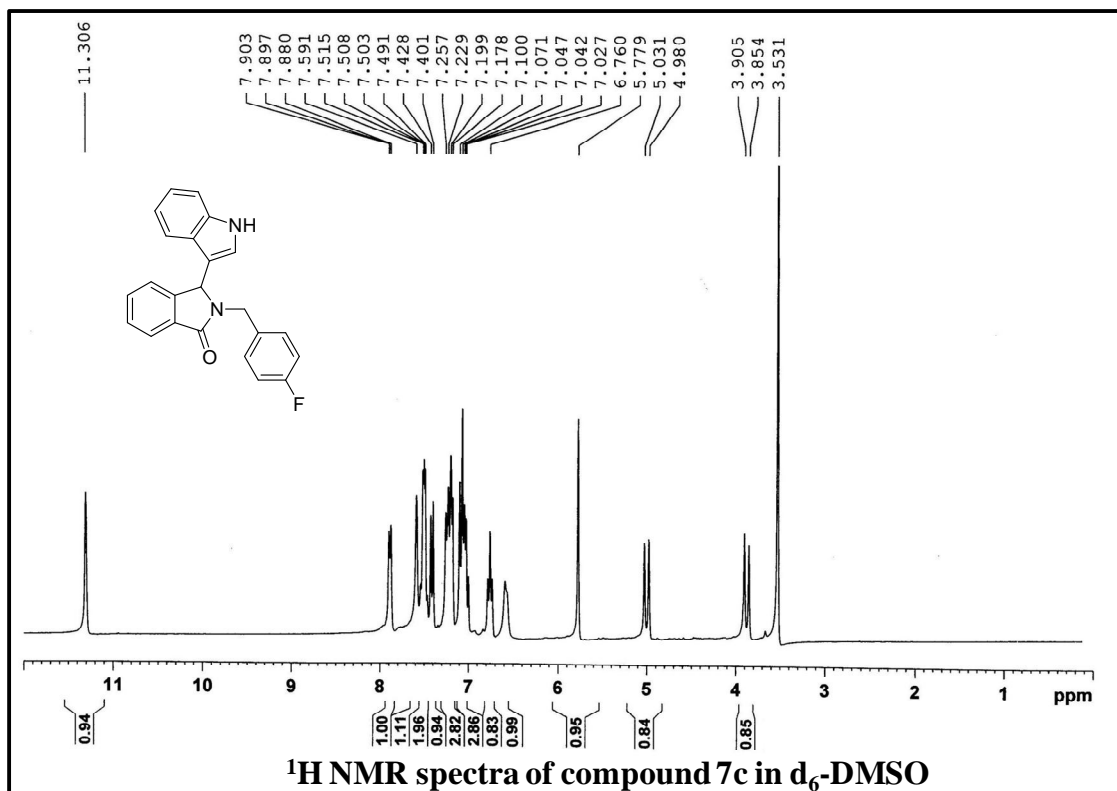
Entry	1	2	3d	7	Yield (%) ^a	Literature m.p [2]/ Observed m.p (°C)
1					78	209.4–211.2/206-208
2					83	200-202
3					84	----
4					80	208.2–208.8/206-208

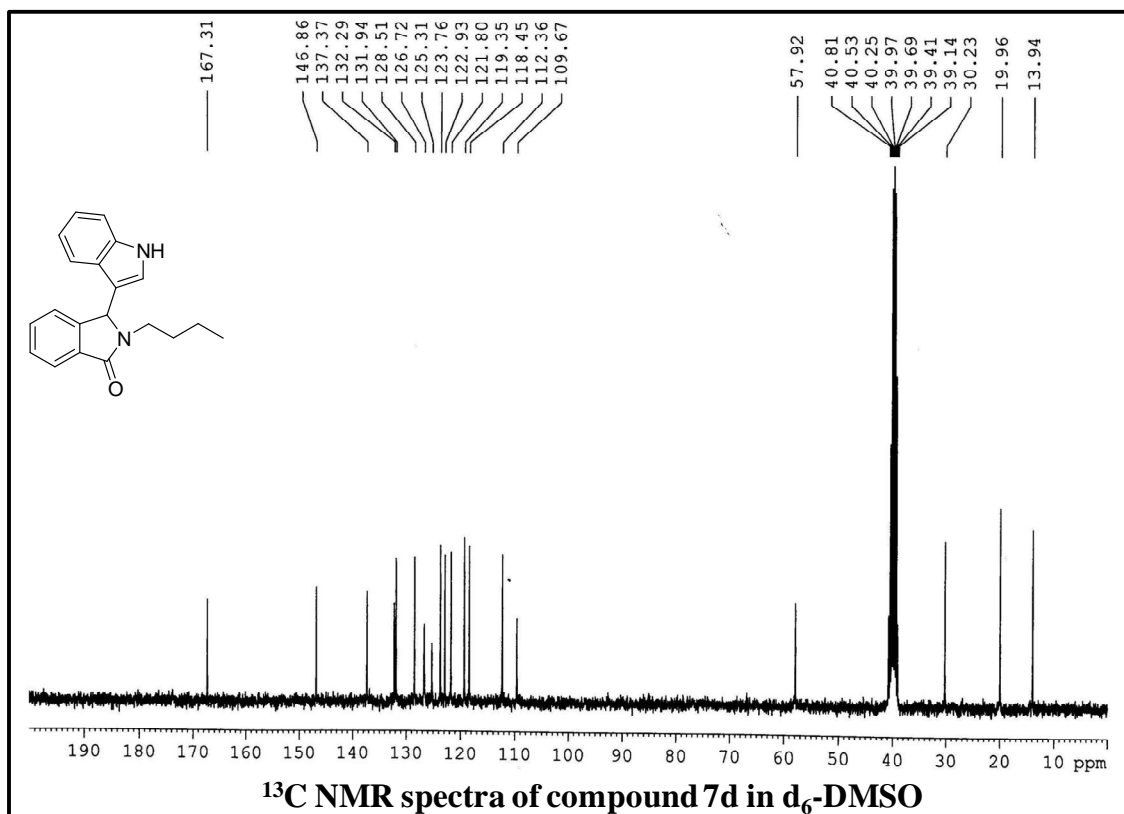
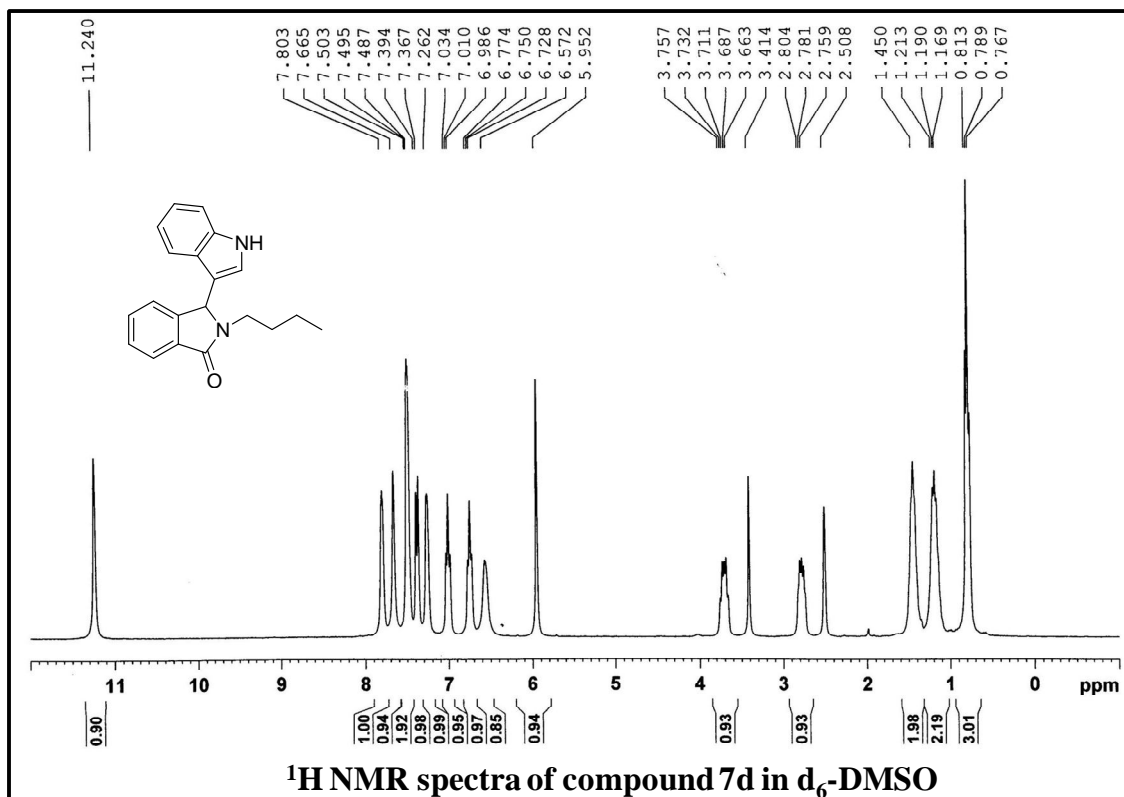
^aIsolated Yield(%)

Spectral data 7a-d:









Preparation of the Catalyst:

Preparation of ZrO₂ nano particle: A solution of ZrO₂Cl₂.8H₂O was condensed under a basic medium (pH ~ 10) at 0–5 °C and the solution was stirred for 24 h at 100°C. The colloidal particles were recovered by centrifugation, washed several times with water, dried and finally, the NPs were calcined at 500 °C for 4 h.³

Infrared spectra: The infrared spectrum of fresh ZrO₂ was depicted in Fig. S1a. The fresh ZrO₂ showed a characteristic broad band at 3453cm⁻¹ and a broad band between 1600-1635 cm⁻¹, which are assigned to the O–H modes of chemisorbed water and/or terminated hydroxides at the surface of the nanoparticles.^{4,5} The infrared spectra of reused catalyst after five runs is depicted in Fig. S1b. It is important to note that all corresponding peaks are intact without any major change in characteristics peak which indicates that structure of catalyst doesn't change even after 5 cycles.

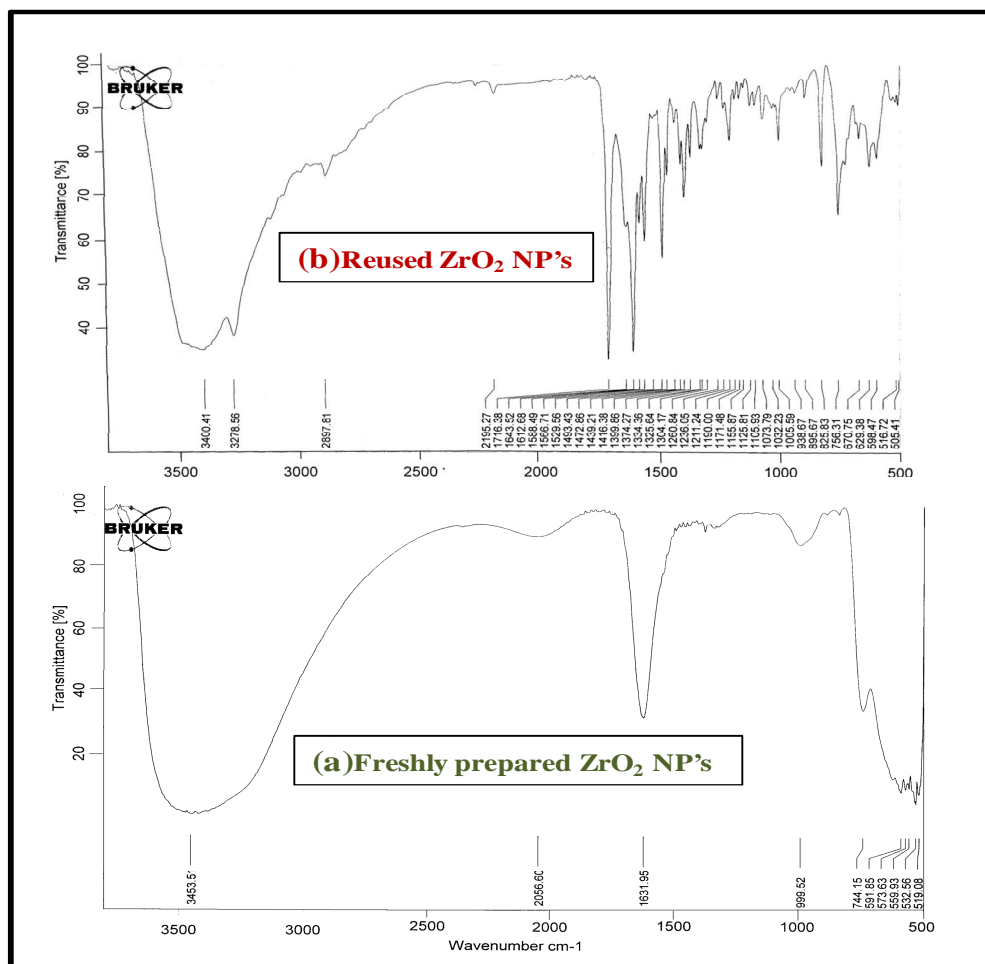


Fig. S1 (a) FT-IR spectra of fresh ZrO_2 NP's and (b) reused ZrO_2 NP's after 5th cycle

References:

1. M. Adib, F. Peytam, M. Zainali, L.-G. Zhu and J. Wub, *Tetrahedron Lett.*, 2015, **56**, 4729.
2. F. Chen, M. Lei and L. Hu, *Green Chem.*, 2014, **16**, 2472.
3. A. Saha, S. Payra and S. Banerjee, *Green Chem.*, 2015, **17**, 2859.
4. K. Nakanishi, *Infrared Absorption Spectroscopy: Practical*, Holden-Day, San Francisco, 1962.
5. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Wiley, New York, 1997.

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